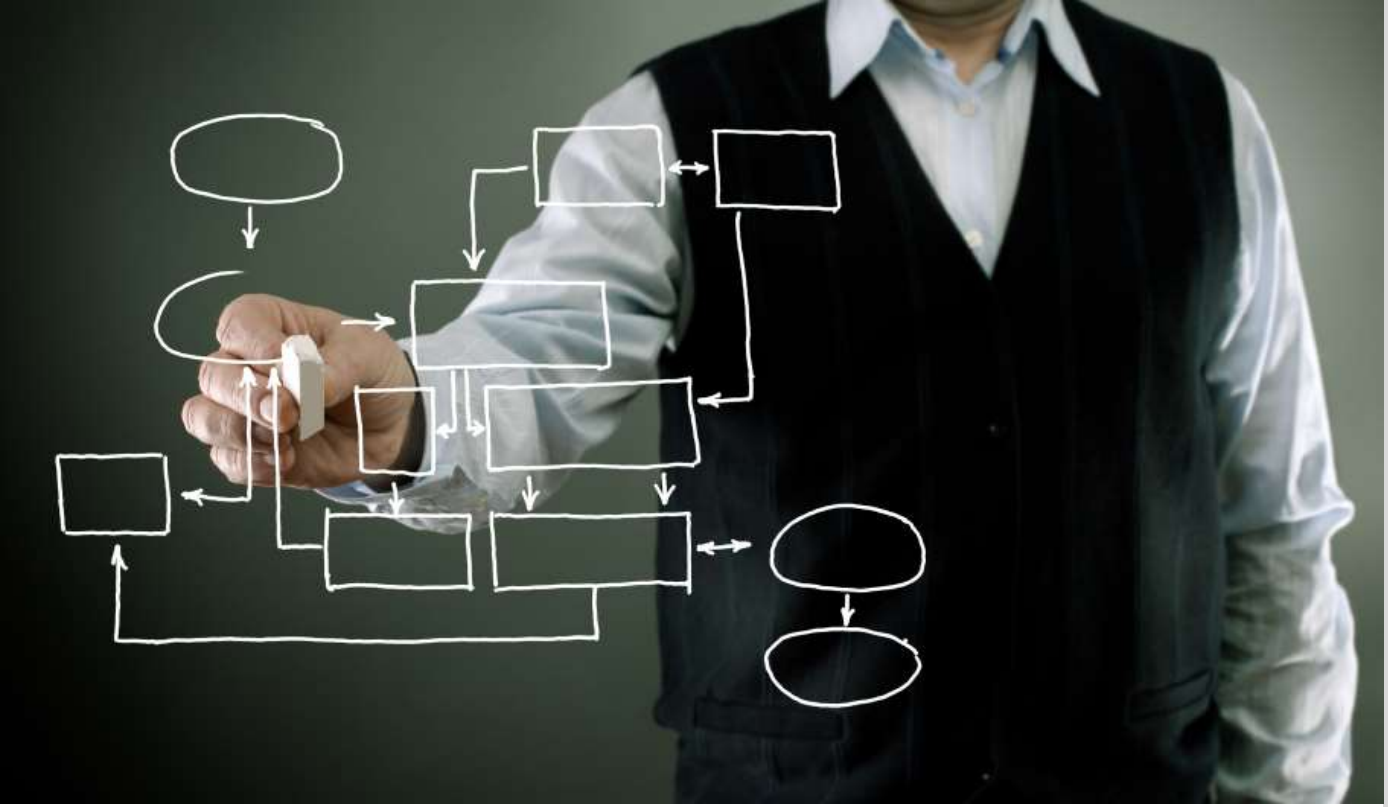

Online Diversity Control in Symbolic Regression via a Fast Hash-based Tree Similarity Measure

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Diversity in Genetic Programming

Diversity represents an important aspect of Genetic Programming

- Describes state of convergence
- Exploration – exploitation trade-off

Many diversity measures for GP [Črepinšek et al., 2013]

- Semantic – phenotypic
- Structural – genotypic
- History-based
- Distance-based
- Difference-based
- Entropy-based
- …

GP Tree Distance

Tree distances seldomly used due to high runtime costs

[Bille, P. (2005). A survey on tree edit distance and related problems. *Theoretical computer science*, *337*(1-3), 217-239.]

- Generally NP-Hard
- At least quadratic in time and space

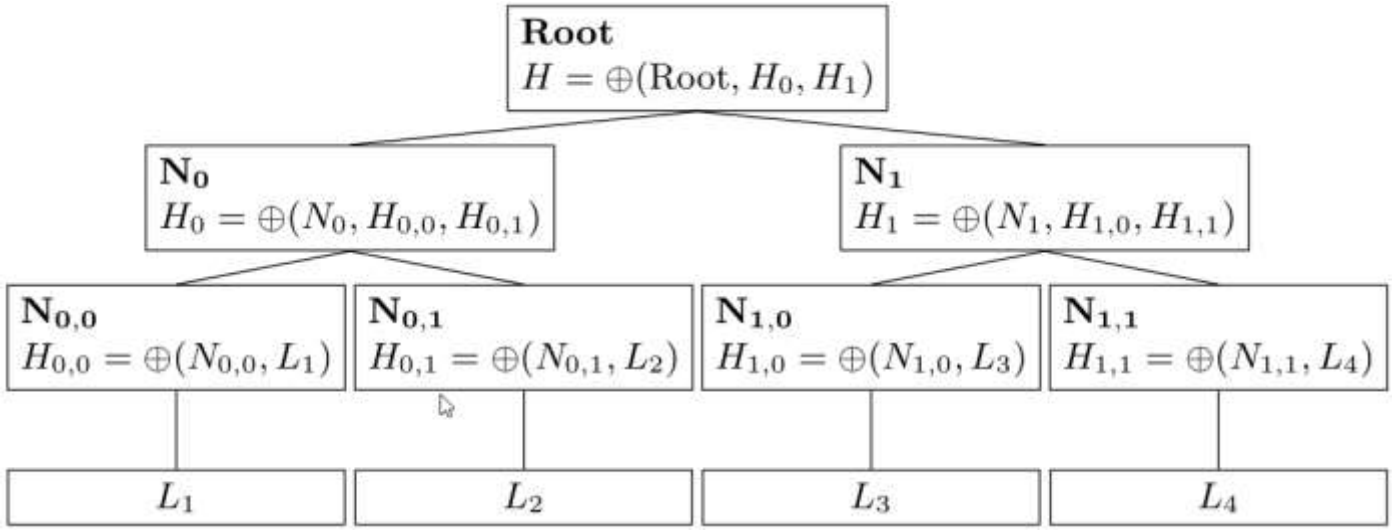
Hash-based tree distance

- Simple algorithm tailored for GP
- Single expensive pass over the population
- Fast calculation of distance matrix
- *Inexact* due to potential hash collisions

Hash-based Tree Distance

Tree hashing algorithm

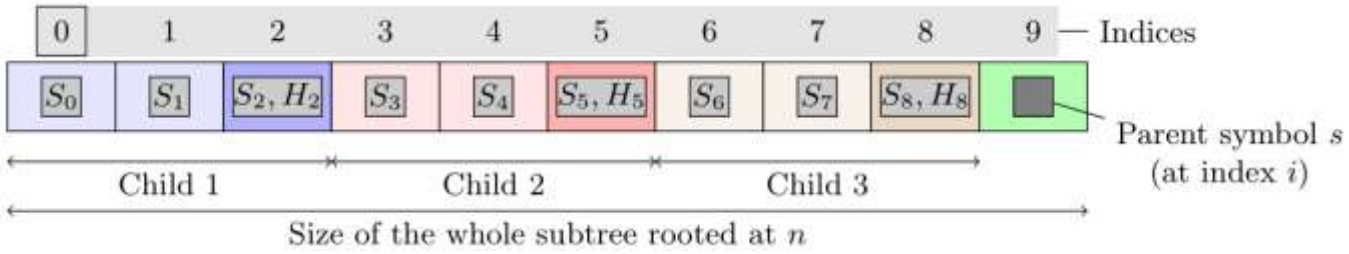
- Converts a tree to a sequence of hash values
- Same hash value → isomorphic subtrees
- Can handle structural and semantic differences
- Parent hash values aggregated from own label + child hash values
- $\oplus$ is a general-purpose hash function (can be cryptographic)



Tree Hashing Algorithm

- **Bottom-up approach**
- **Sort commutative symbols**
- **Hashing mode:**
  - Structural: only hash node labels ($Constant, X_1, Y$, etc.)
  - Hybrid: hash numerical coefficients ($3.14, 3 \cdot X_1, 0.6 \cdot Y$, etc.)

- **Simple array operations**



Hash-based Tree Distance

Distance defined as ratio of common hash values

- Sørensen–Dice coefficient returns a value in $[0,1]$
- M is a mapping of isomorphic subtrees (same hash value)
- M computed as the intersection of corresponding hash value sequences H_1, H_2

$$S(T_1, T_2) = \frac{2 \cdot |M|}{|T_1| + |T_2|} \text{ (tree similarity)}$$
$$D(T_1, T_2) = 1 - S(T_1, T_2) \text{ (tree distance)}$$

Single hashing pass over GP population

- Hash each tree into corresponding hash value sequence
- Sort all hash value sequences
- Simple merge-count to calculate tree distance

Hash-based Tree Distance

Runtime performance

- Identical results to bottom-up tree distance [Valiente, 2001]
- Compute distance matrix for 5000 random trees
- Single-mode: hash each tree anew when computing distance matrix
- Batch-mode: hash and sort all trees, use hash value sequences for further computation

TABLE I
RUNTIME PERFORMANCE OF HASH-BASED TREE DISTANCE VS THE BOTTOM-UP TREE DISTANCE

Tree distance method	Elapsed time (s)	Speed-up
Bottom-up	1225.751	1.0x
Hash-based (single-mode)	297.521	4.1x
Hash-based (batch-mode)	3.677	333.3x

Suitable for online diversity control

Online Diversity Control

Approach

- Compute distance matrix per generation
- Favor individuals that are “farther away”

Implementation

- Standard GA: average distance as penalty to fitness (during selection)
- NSGA-II: maximize average distance as secondary objective

Secondary objectives

- Structural and hybrid distance
- Recursive complexity
- Tree size
- Visitation length
- Number of variables

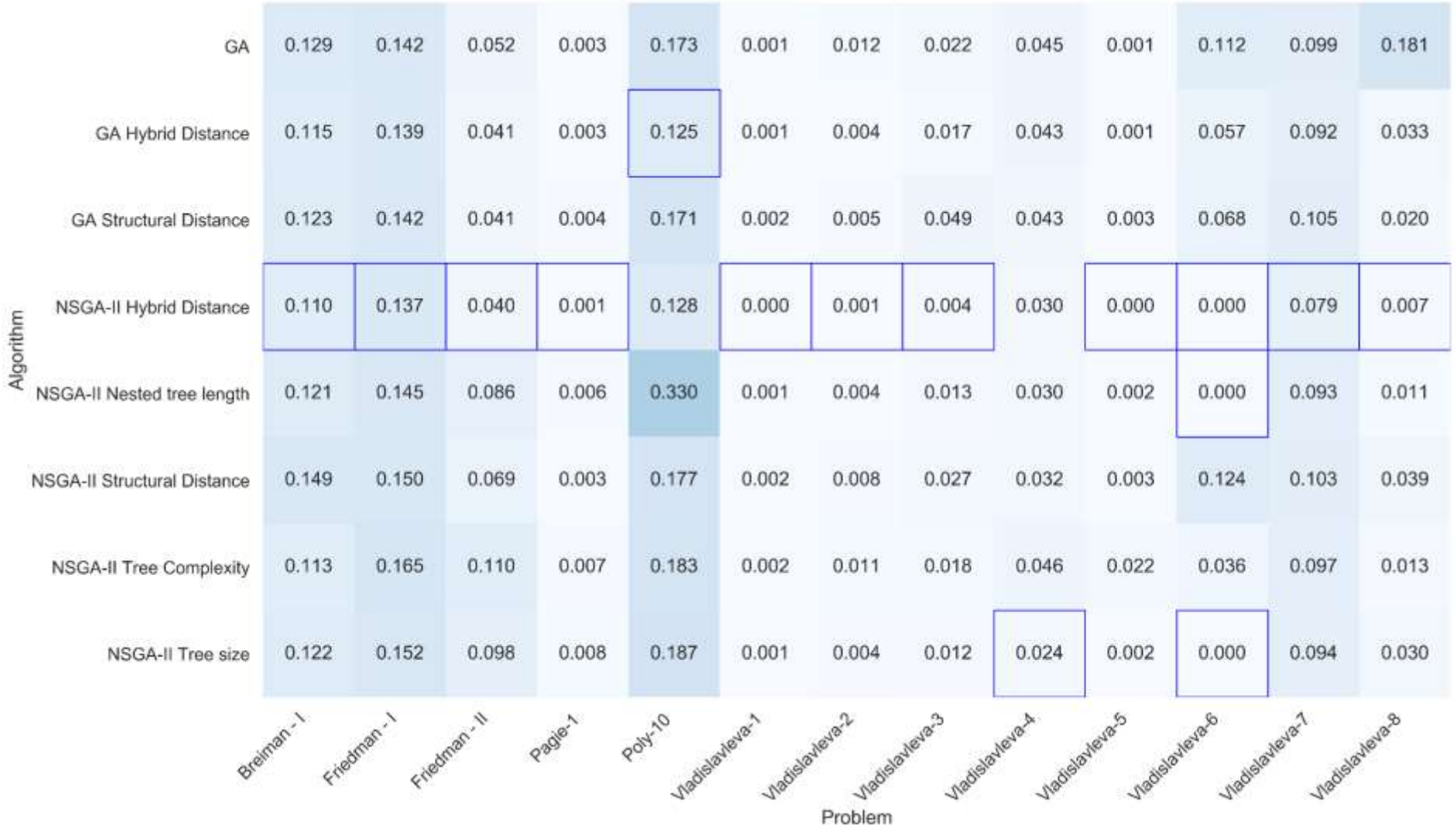
Performance Ranking

Median rank over all problems

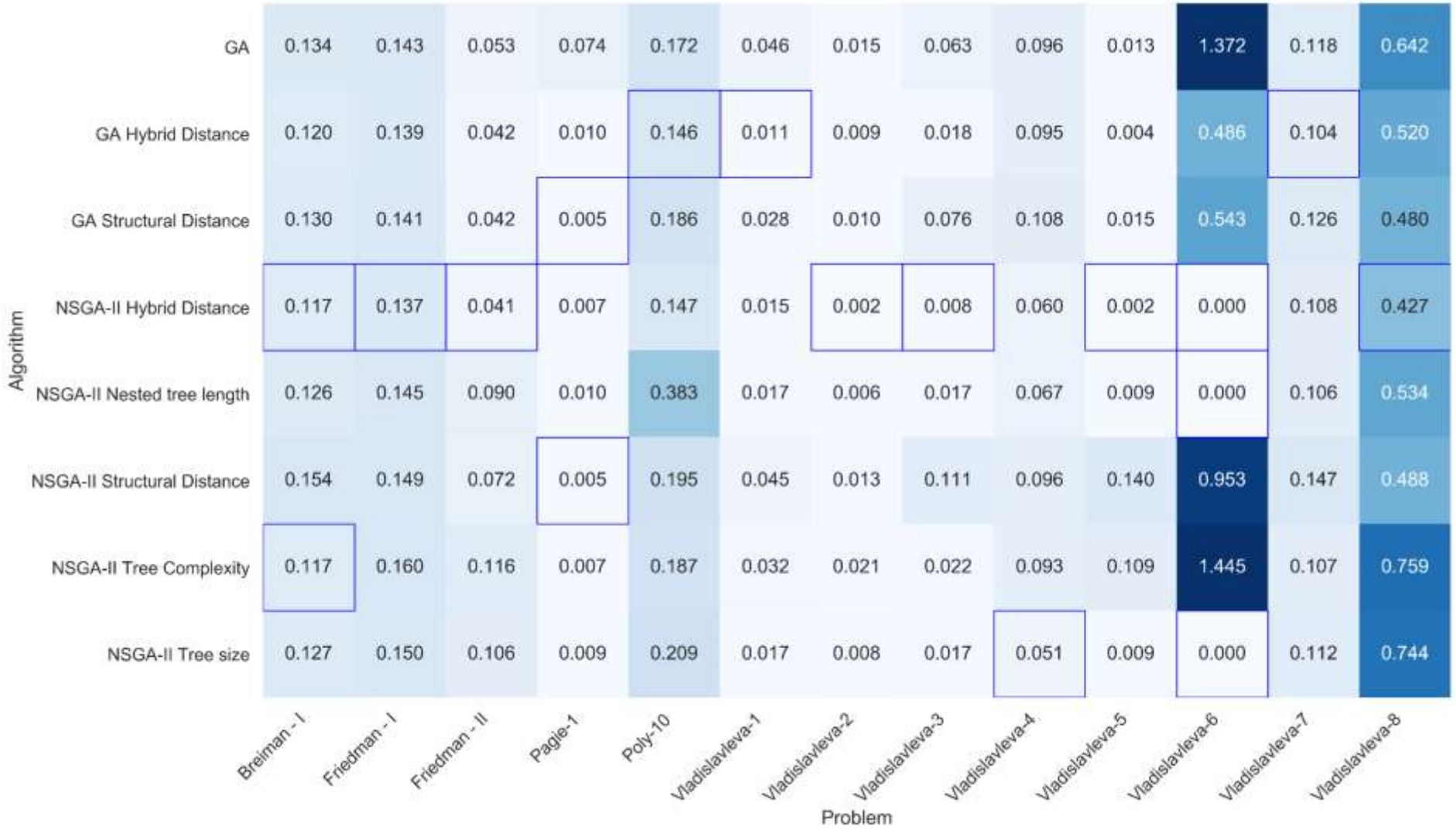
- NSGA-II Hybrid and GA Hybrid overall best
- NSGA-II Hybrid produces higher quality and lower result variance

Algorithm	Training rank	Test rank
NSGA-II Hybrid distance	1.0	1.0
GA Hybrid distance	2.0	3.0
NSGA-II Nested tree size	4.0	4.0
GA Structural distance	5.0	5.0
NSGA-II Tree size	5.0	5.0
GA Standard	6.0	6.0
NSGA-II Tree complexity	6.0	6.0
NSGA-II Structural distance	7.0	6.0

Normalized Mean Squared Error (Train)

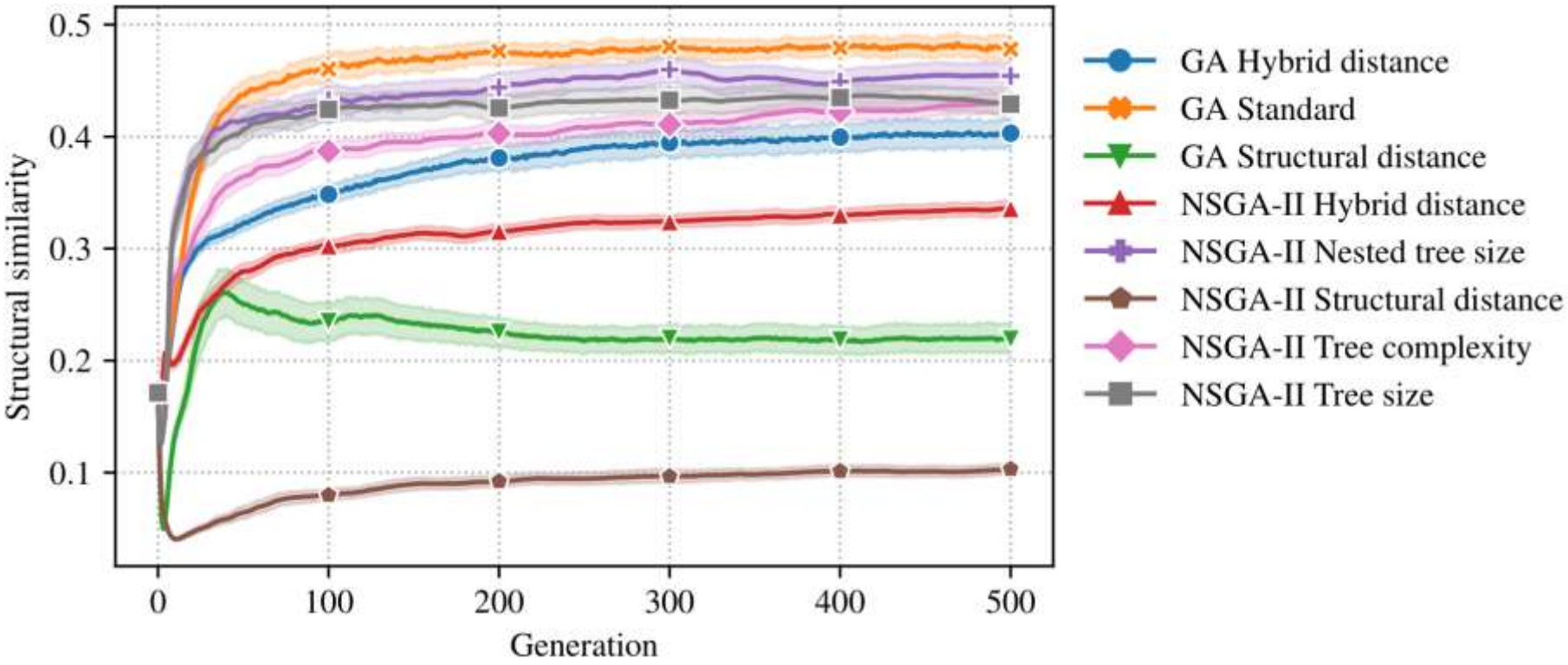


Normalized Mean Squared Error (Test)



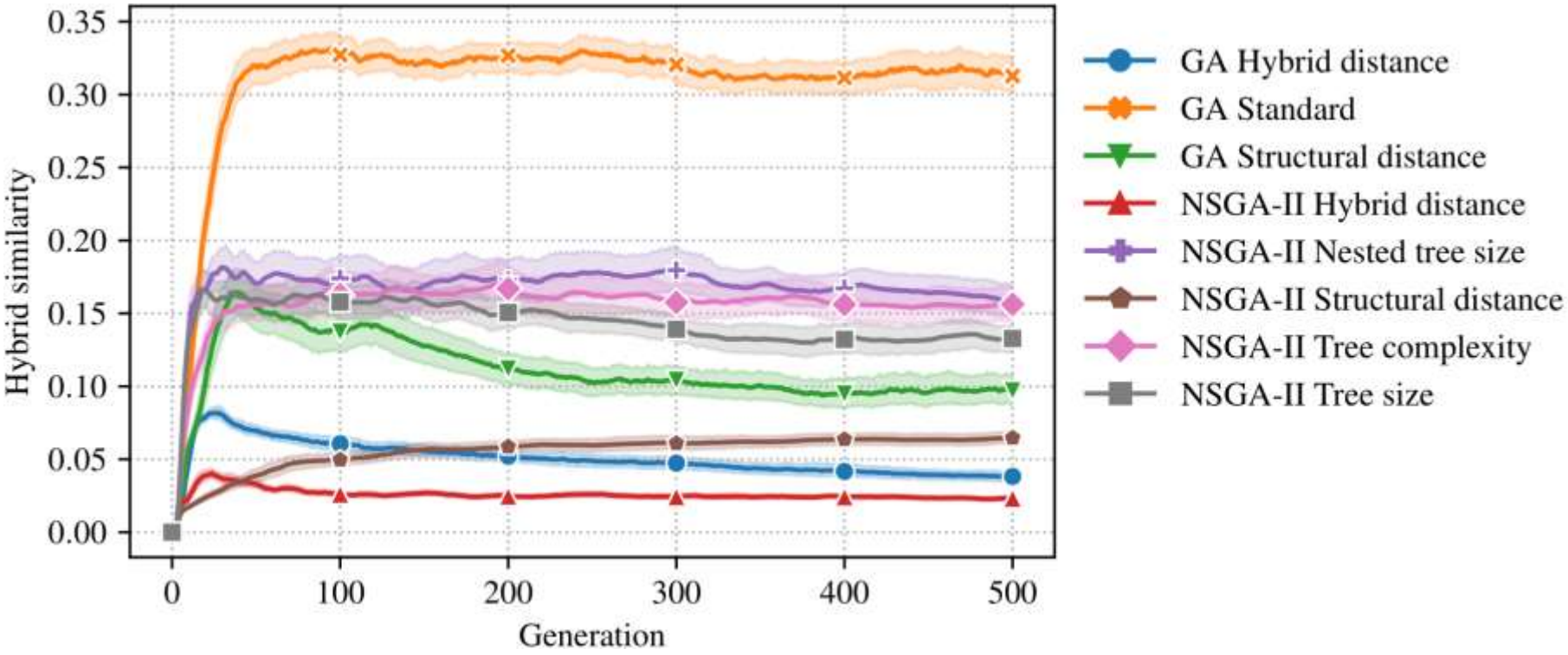
Evolution of Diversity

- Structural similarity $S = 1 - D$



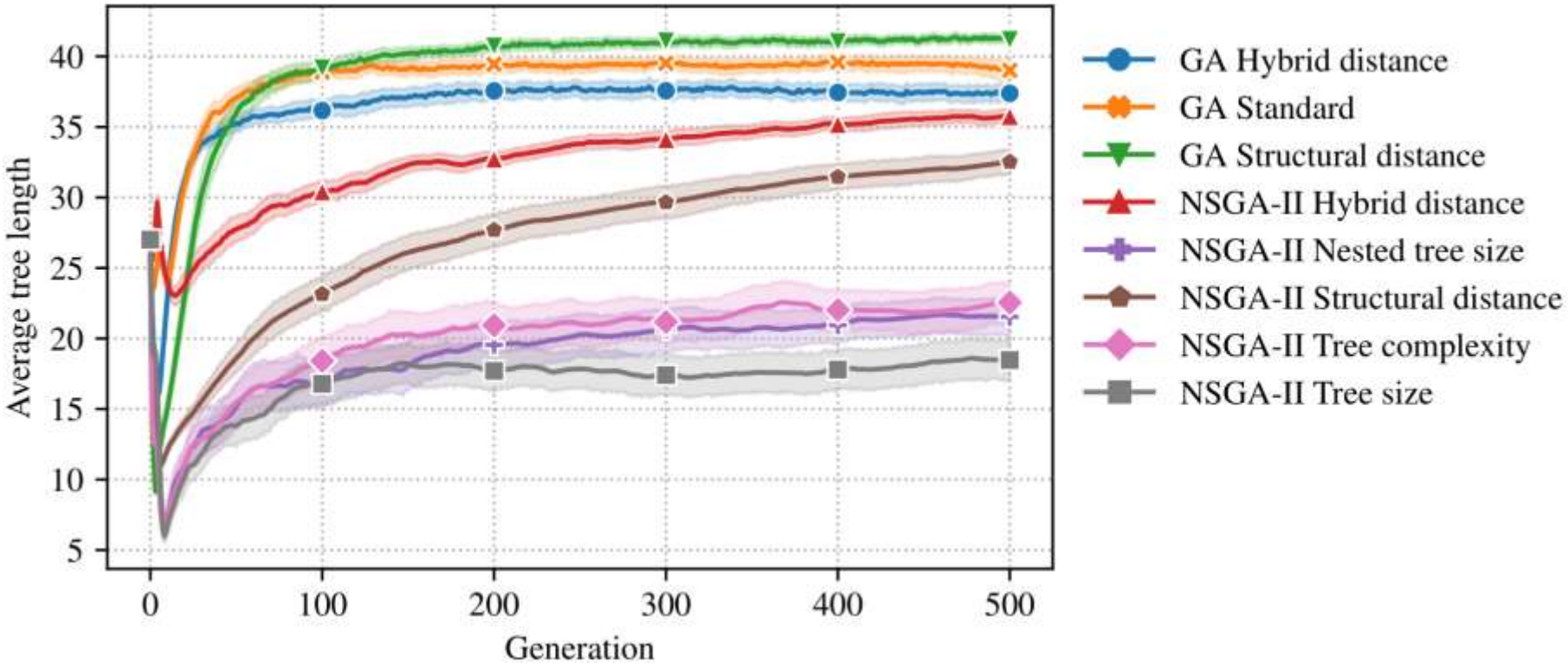
Evolution of Diversity

- Hybrid similarity $S = 1 - D$



Evolution of Tree Length

Average tree length



Runtime Analysis

Distance computation overhead

Algorithm	Runtime (s)
Poly-10 (250 training rows)	
GA Standard (baseline)	160.1
GA Hybrid distance	285.1
GA Structural distance	301.9
NSGA-II Hybrid distance	317.5
NSGA-II Structural distance	293.1
NSGA-II Complexity	195.5
NSGA-II Nested Tree Length	196.5
NSGA-II Tree Length	189.8
Breiman-I (5000 training rows)	
GA Standard (baseline)	899.3
GA Hybrid distance	1034.9
GA Structural distance	1204.1
NSGA-II Hybrid distance	1092.0
NSGA-II Structural distance	1140.6
NSGA-II Complexity	830.4
NSGA-II Nested Tree Length	842.0
NSGA-II Tree Length	820.3

Summary

Hash-based tree distance for GP

- Computationally-efficient
- Semantically-aware
- Hash-value sequences → mining of common patterns and building blocks
- Easy to integrate with other GP flavors or other operators (e.g. Crossover)
- Open-source: https://dev.heuristiclab.com/

Online diversity control

- Feasible for large populations
- Proof of concept successfully compares to other GP variants

Future research

- More sophisticated diversity tuning
- Detailed analysis of diversity
- Mining of common subtrees

Discussion

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