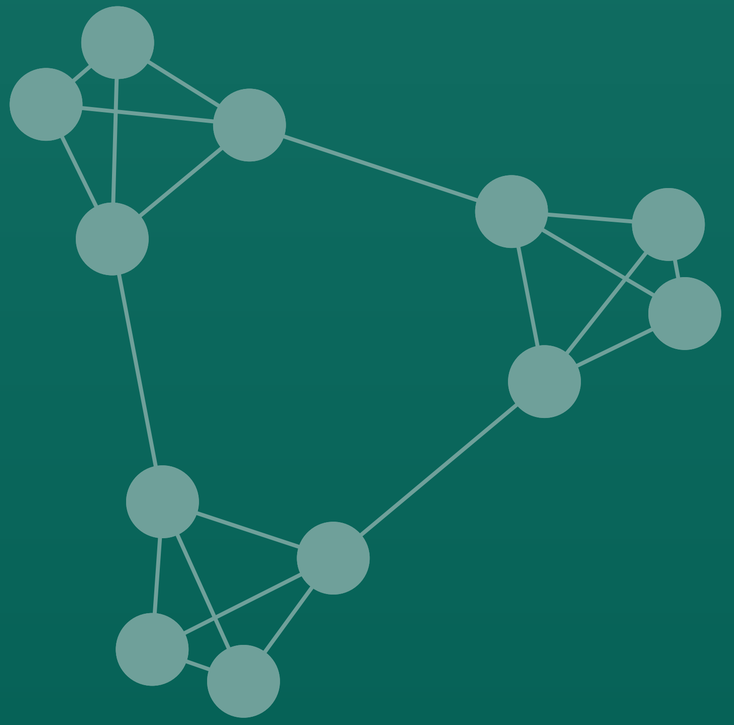
No Metric to Rule Them All



Toward Principled Evaluations
of Graph-Learning Datasets

The Fellowship

Corinna Coupette

Jeremy Wayland

Emily Simons

Bastian Rieck

Coupette*, Wayland*, Simons, and Rieck. *No Metric to Rule Them All.* ICML 2025.

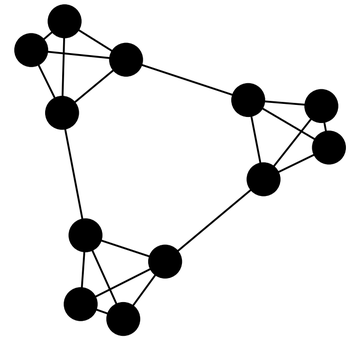
Graph Learning Benchmarks need a reality check.

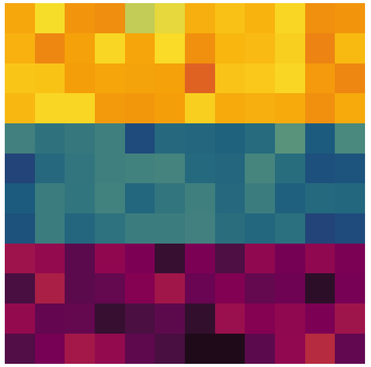
Coupette*, Wayland*, Simons, and Rieck. *No Metric to Rule Them All.* ICML 2025.

Guiding Questions

Q1: What characterizes a good graph-learning dataset?

Q2: How can we evaluate dataset quality in graph learning?





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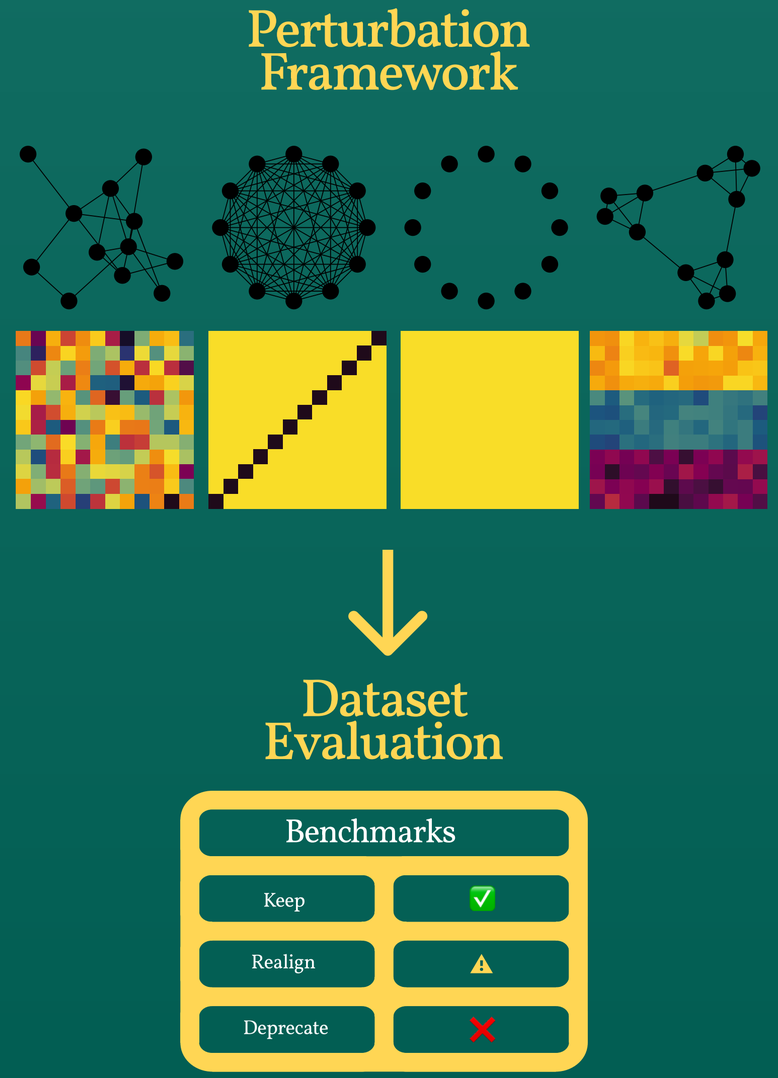
RINGS

Relevant **I**nformation in **N**ode features and **G**raph **S**tructure



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Guiding Principles

P1: *Task-Relevant Information*
→ Both structure and features should matter for a given task.

P2: *Complementary Information*
→ Structure and features should offer distinct views of the data.

Associated Metric

Performance separability

Mode complementarity

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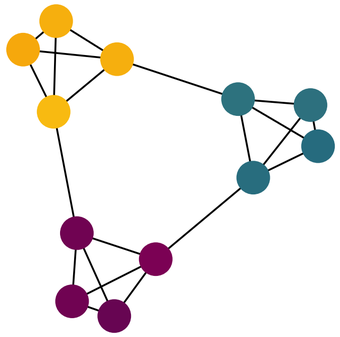
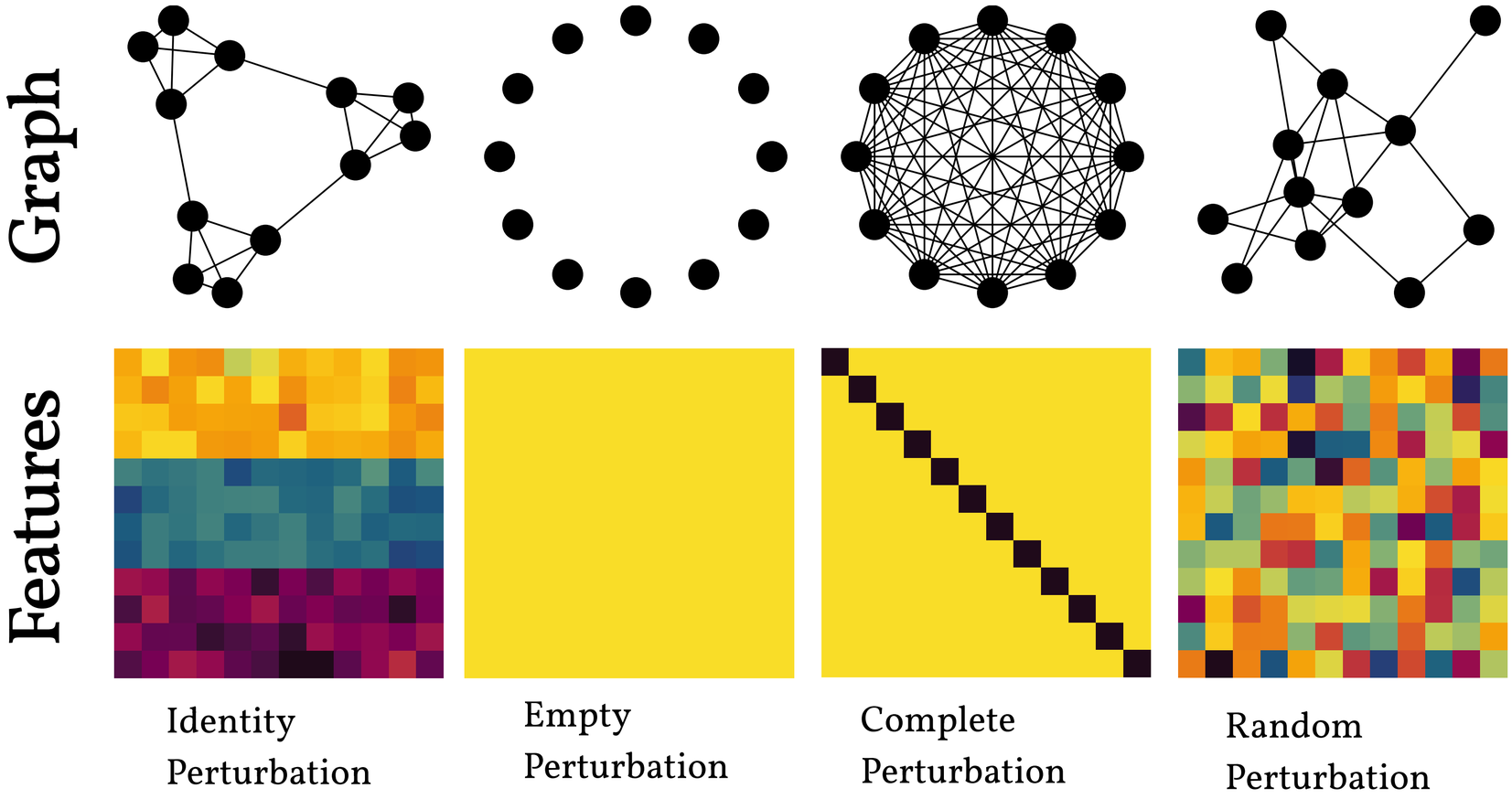


Mode Perturbations



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Performance Separability

A Task-Dependent Measure

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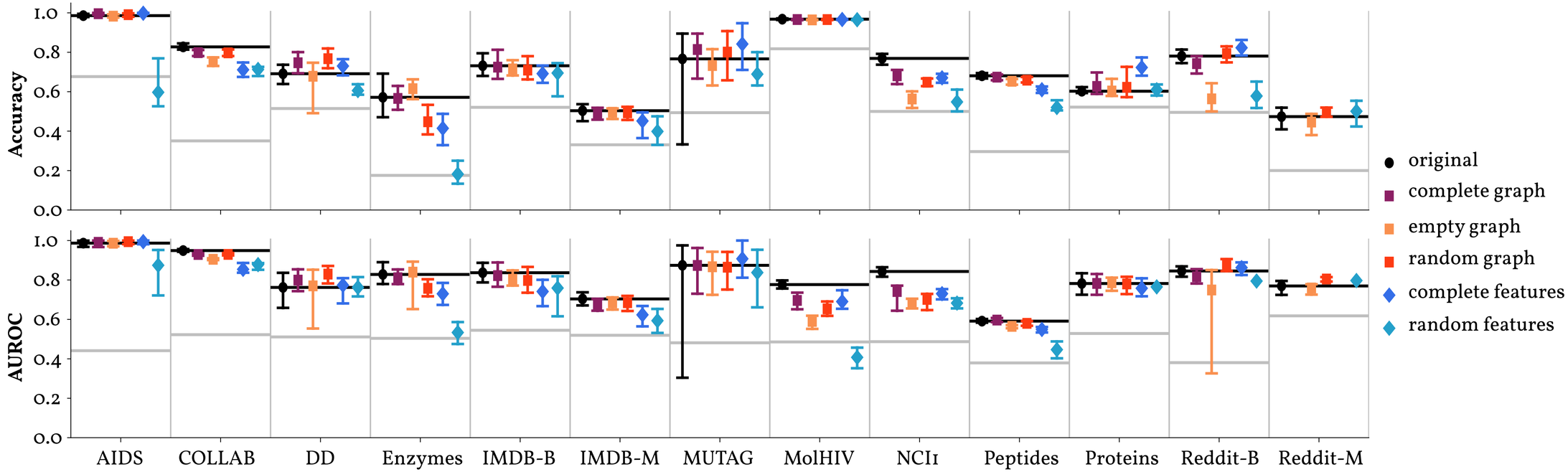
Many popular datasets fail to statistically outperform their perturbed versions.



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Mode Complementarity

A Task-Independent Measure

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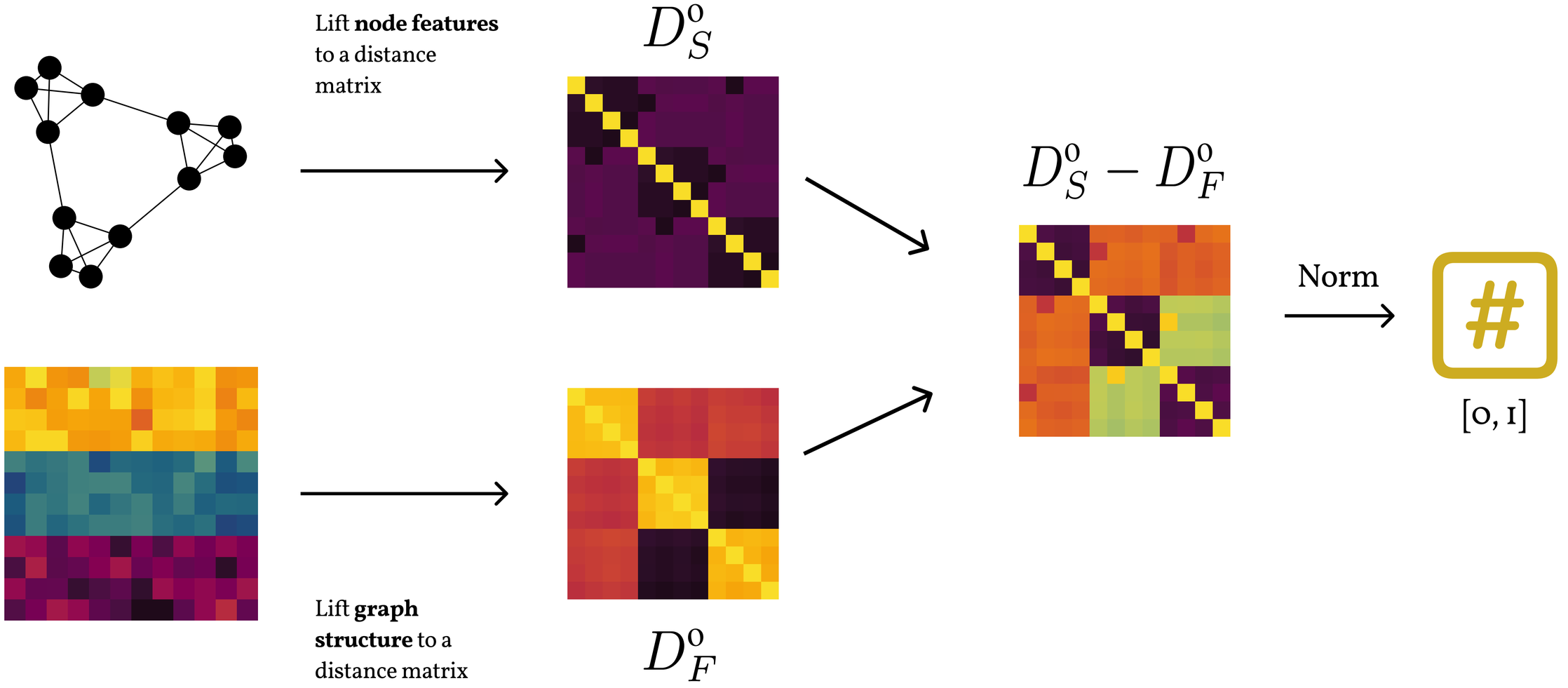
Calculating Mode Complementarity



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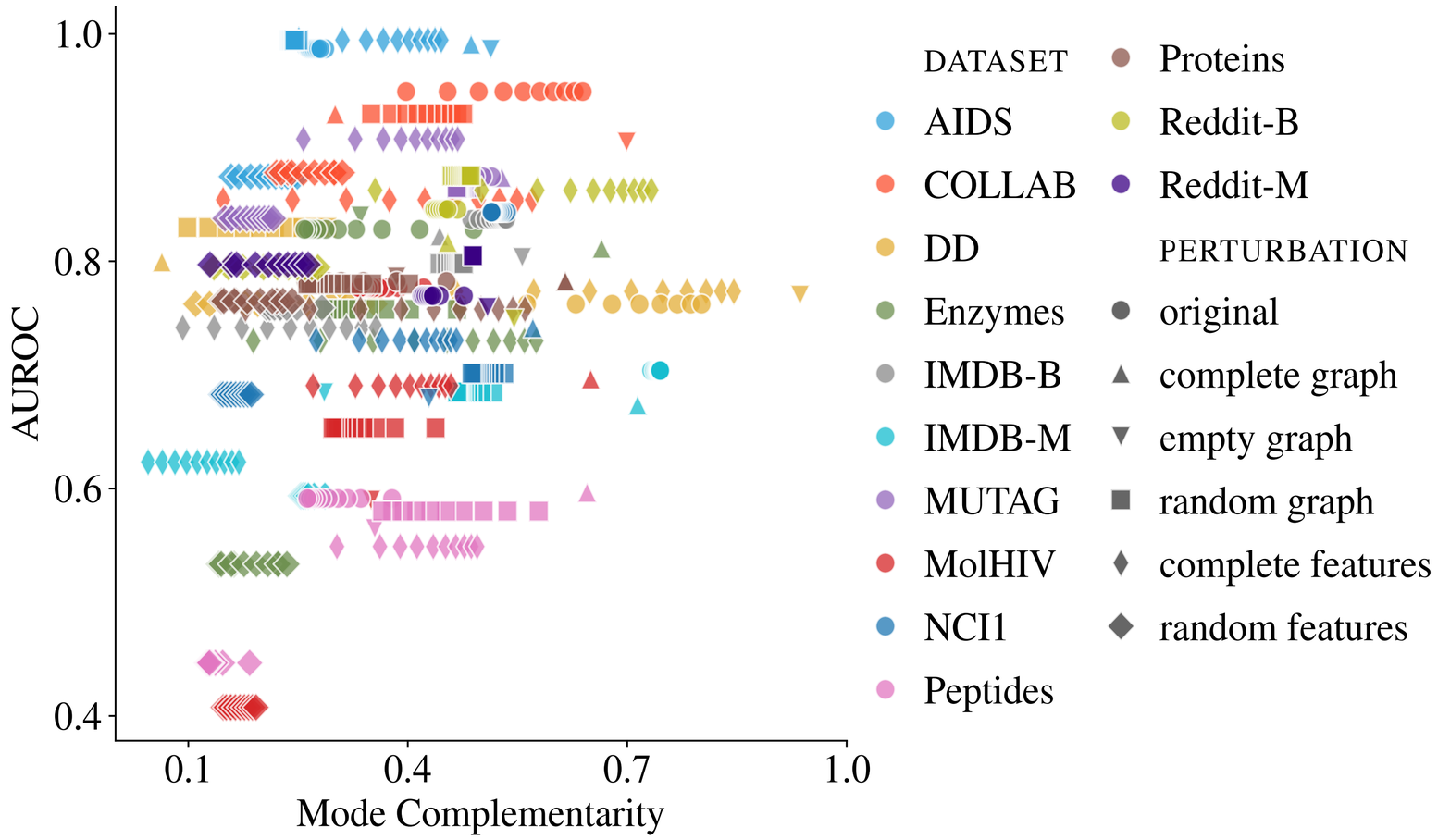
Mode complementarity correlates with performance.



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Mode Diversity

A Task-Independent Measure

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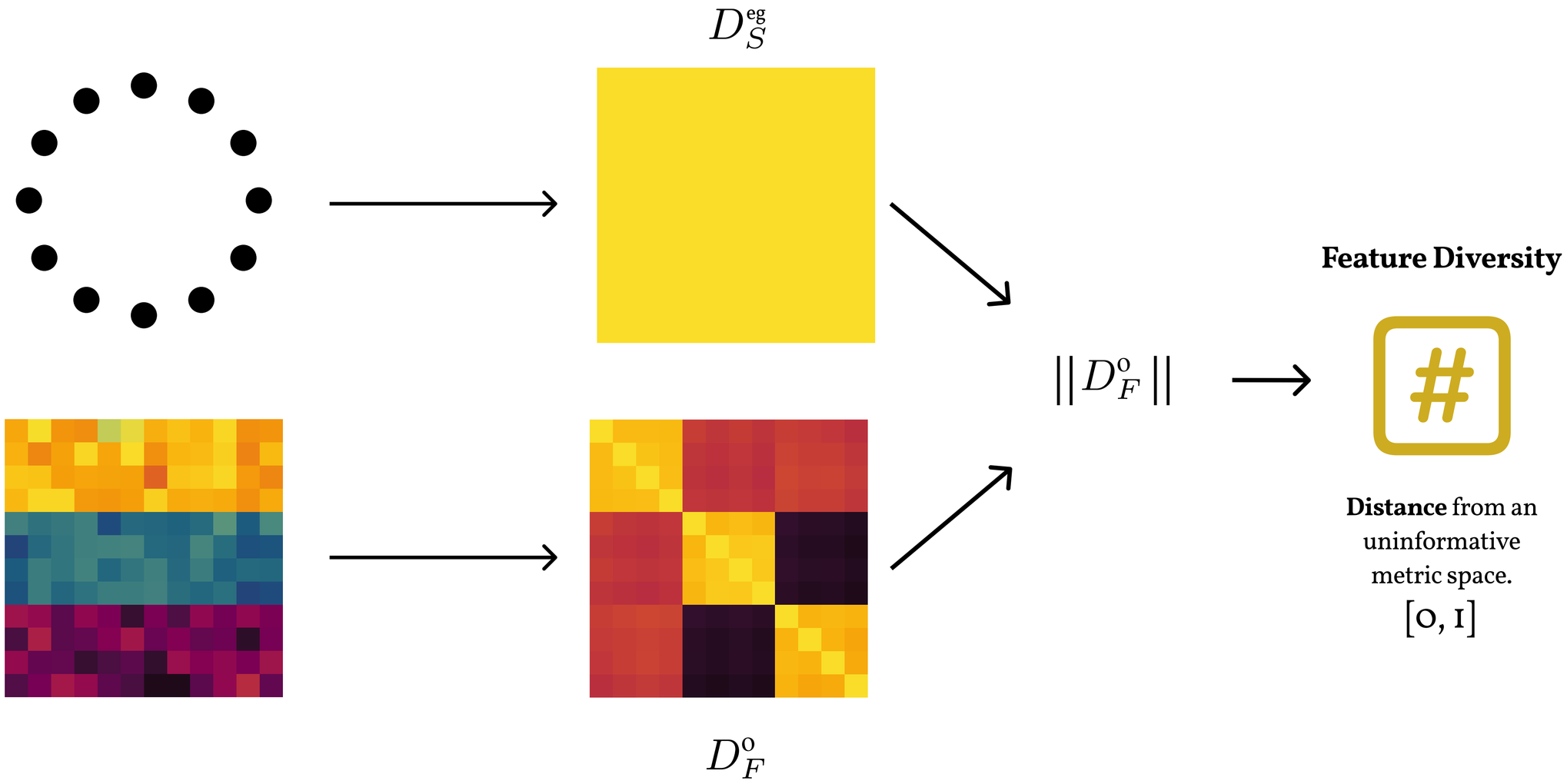
Calculating Feature Mode Diversity



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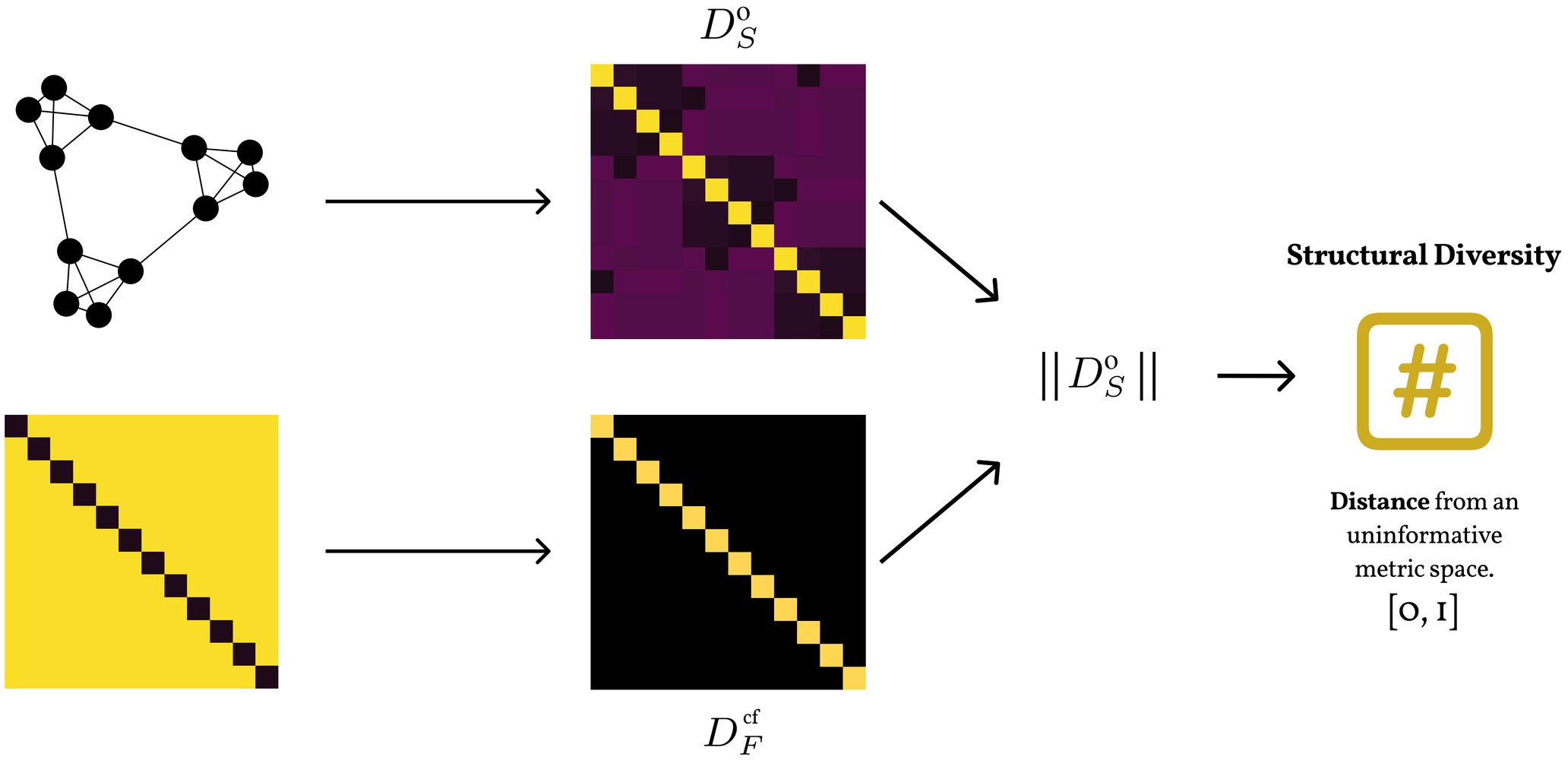
Calculating Structural Mode Diversity



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Final Evaluation

A Benchmark Taxonomy

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Result Overview

Dataset	Performance Separability (†)			Mode Diversity (‡)		Action
	Structure	Features	Overall	Structure (μ:σ)	Features (μ:σ)	
MolHIV	+	+	++	○:−−	++:++	Keep (†|‡)
NCI1	+	+	++	○:−−	++:++	
Peptides	○	+	+	++:−−	++:++	
AIDS	−	−	−−	○:−	++:○	Realign (†|‡)
DD	−	−	−−	++:−	−−:−−	
MUTAG	○	−	−	○:−−	++:○	
Reddit-{B,M}	−	−	−−	++:−−	++:○	
COLLAB	+	+	++	−:++	−:++	Deprecate (‡)
IMDB-B	○	○	○	−−:○	○:++	
IMDB-M	○	+	+	−−:○	−:++	
Enzymes	−	+	−	−:−	++:○	Deprecate (†|‡)
Proteins	−	−	−−	−:○	++:−	

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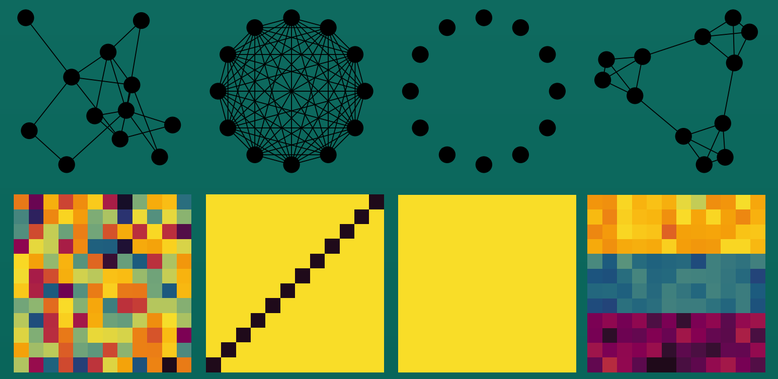
Relevant **I**nformation in **N**ode features and **G**raph **S**tructure

Perturbation Framework



Desiderata

Both modes should matter for a given task. → **Performance Separability**

Modes should offer distinct and interesting views of the data. → **Mode Complementarity & Mode Diversity**

Metrics

Dataset Evaluation

Benchmarks	
Keep	✅
Realign	⚠
Deprecate	❌

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