# Diversity Curves for Graph Representation Learning

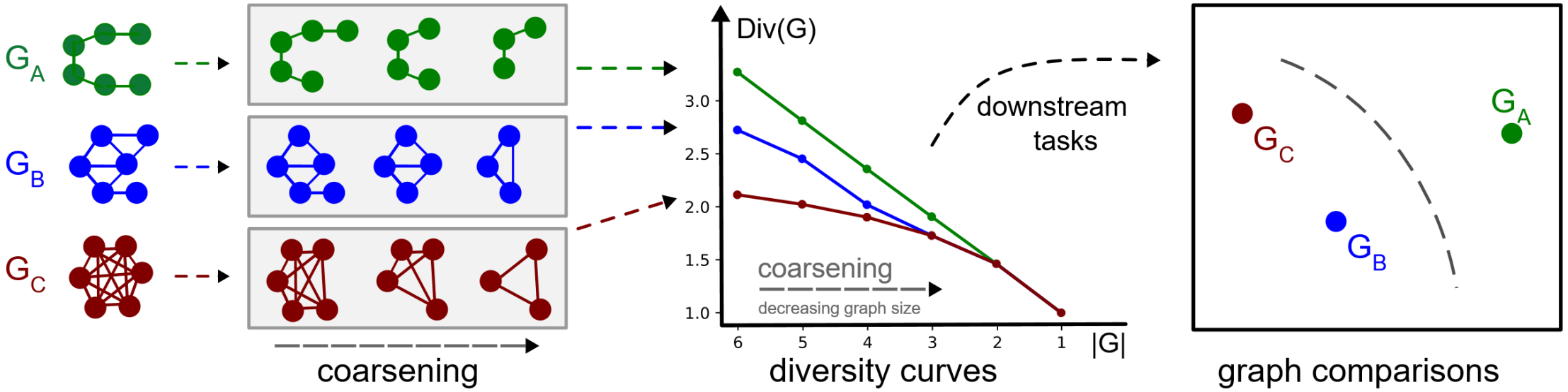
Katharina Limbeck, Nadja Häusermann, Martin Carrasco,
Guy Wolf‡, Bastian Rieck‡

Paper

Code

# Diversity curves as graph representations

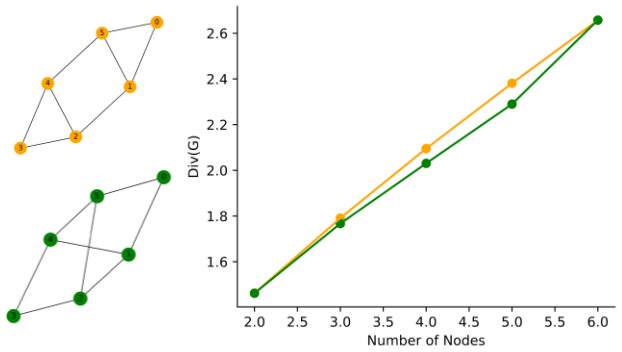
We propose **diversity curves**, novel graph-level representations for unsupervised tasks that track **structural diversity**, the spread of graphs, across edge-contraction **coarsening levels**.



# It works!

Diversity curves **behave well** in theory and in simulated experiments, particularly they…

increase expressivity through coarsening




detect perturbations



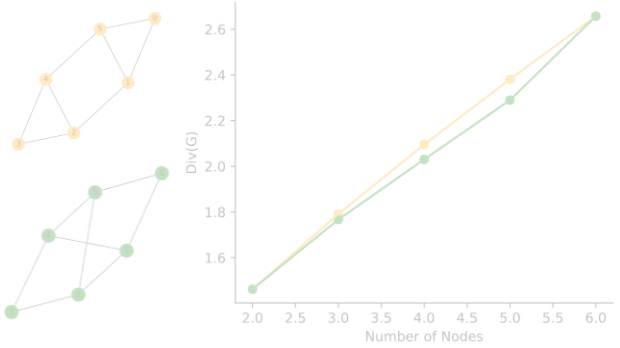

distinguishing graph distributions

| Method | Accuracy (↑) | Silhouette Score (↑) |
|---|---|---|
| Diversity Curves (ours) | **0.90 ± 0.06** | **0.42 ± 0.03** |
| Kernel WL Opt. Assig. | **0.90 ± 0.05** | 0.02 ± 0.00 |
| Kernel Shortest Path | 0.77 ± 0.07 | 0.28 ± 0.04 |
| TopER | 0.70 ± 0.10 | −0.06 ± 0.02 |
| NetLSD | 0.90 ± 0.03 | 0.06 ± 0.04 |
| FEATHER | 0.75 ± 0.09 | 0.11 ± 0.02 |
| Spectral Zoo | 0.72 ± 0.09 | 0.05 ± 0.03 |
| PH Vietoris–Rips | 0.78 ± 0.07 | −0.01 ± 0.03 |

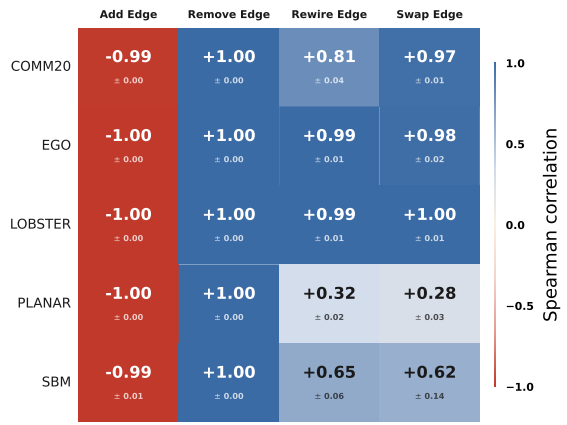
# It works!

Diversity curves **behave well** in theory and in simulated experiments, particularly they…

## increase expressivity through coarsening




## detect perturbations



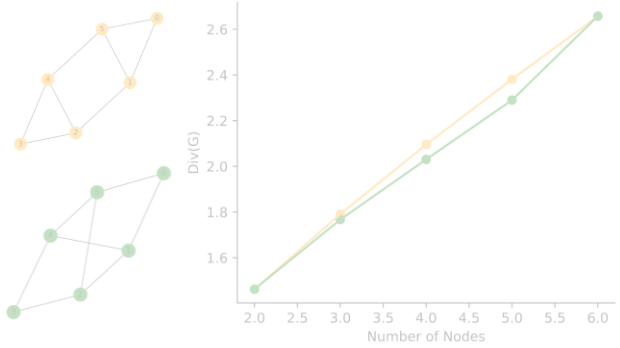

## distinguishing graph distributions

| Method | Accuracy (↑) | Silhouette Score (↑) |
|---|---|---|
| Diversity Curves (ours) | **0.90 ± 0.06** | **0.42 ± 0.03** |
| Kernel WL Opt. Assig. | **0.90 ± 0.05** | 0.02 ± 0.00 |
| Kernel Shortest Path | 0.77 ± 0.07 | 0.28 ± 0.04 |
| TopER | 0.70 ± 0.10 | −0.06 ± 0.02 |
| NetLSD | 0.90 ± 0.03 | 0.06 ± 0.04 |
| FEATHER | 0.75 ± 0.09 | 0.11 ± 0.02 |
| Spectral Zoo | 0.72 ± 0.09 | 0.05 ± 0.03 |
| PH Vietoris–Rips | 0.78 ± 0.07 | −0.01 ± 0.03 |

# It works!

Diversity curves **behave well** in theory and in simulated experiments, particularly they…

### increase expressivity through coarsening




### detect perturbations



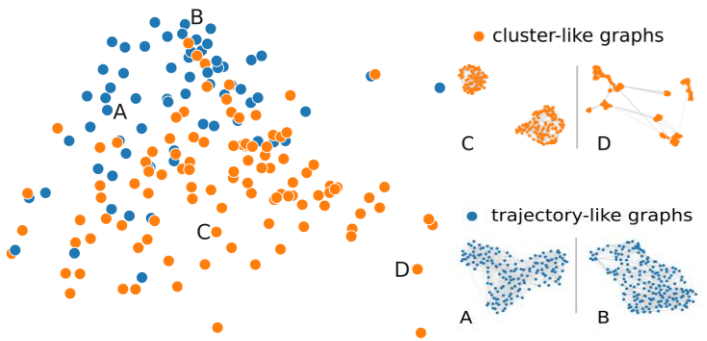

### distinguish graph distributions

| Method | Accuracy (↑) | Silhouette Score (↑) |
|---|---|---|
| Diversity Curves (ours) | **0.90 ± 0.06** | **0.42 ± 0.03** |
| Kernel WL Opt. Assig. | **0.90 ± 0.05** | 0.02 ± 0.00 |
| Kernel Shortest Path | 0.77 ± 0.07 | 0.28 ± 0.04 |
| TopER | 0.70 ± 0.10 | −0.06 ± 0.02 |
| NetLSD | 0.90 ± 0.03 | 0.06 ± 0.04 |
| FEATHER | 0.75 ± 0.09 | 0.11 ± 0.02 |
| Spectral Zoo | 0.72 ± 0.09 | 0.05 ± 0.03 |
| PH Vietoris–Rips | 0.78 ± 0.07 | −0.01 ± 0.03 |

# It works!

Diversity curves are **robust to graph size** while performing well on a variety of applications and ...

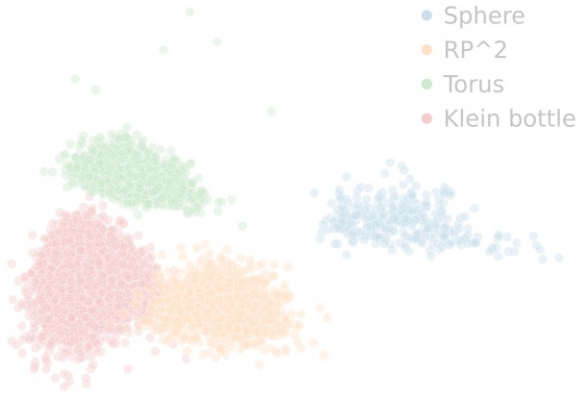
distinguish single-cell graphs




characterise molecular graph datasets



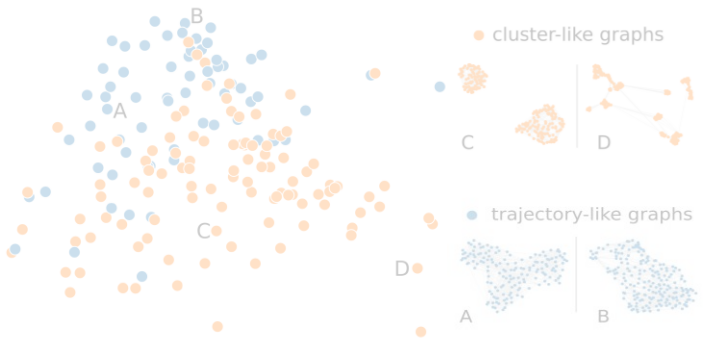

encode geometric shapes



# It works!

Diversity curves are **robust to graph size** while performing well on a variety of applications and ...

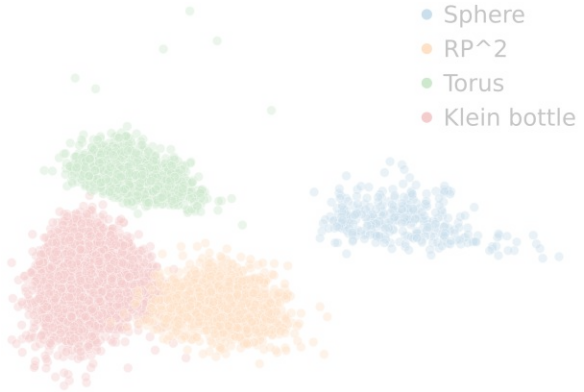
distinguish single-cell graphs




characterise molecular graph datasets

| enzyme graphs | ENZYMES | | | | PROTEINS | | | |
|---|---|---|---|---|---|---|---|---|
| Hydrolases (EC 3) | 1 | 0.46 | 0.6 | 0.72 | 0.002 | 0.001 | 0.001 | 0.001 |
| Ligases (EC 6) | 0.46 | 1 | 0.67 | 0.71 | 0.036 | 0.002 | 0.002 | 0.001 |
| Isomerases (EC 5) | 0.6 | 0.67 | 1 | 0.82 | 0.026 | 0.001 | 0.001 | 0.001 |
| Transferases (EC 2) | 0.72 | 0.71 | 0.82 | 1 | 0.019 | 0.001 | 0.001 | 0.001 |
| Oxidoreductases (EC 1) | 0.002 | 0.036 | 0.026 | 0.019 | 1 | 0.24 | 0.21 | 0.001 |
| Lyases (EC 4) | 0.001 | 0.002 | 0.001 | 0.001 | 0.24 | 1 | 0.45 | 0.001 |
| Enzymes | 0.001 | 0.002 | 0.001 | 0.001 | 0.21 | 0.45 | 1 | 0.001 |
| Non-enzymes | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 0.001 | 1 |

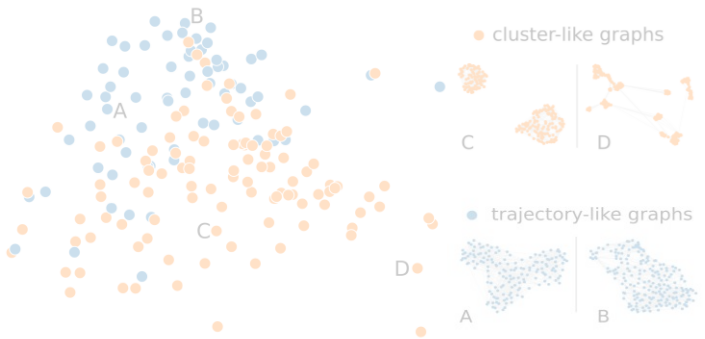
encode geometric shapes



# It works!

Diversity curves are **robust to graph size** while performing well on a variety of applications and ...

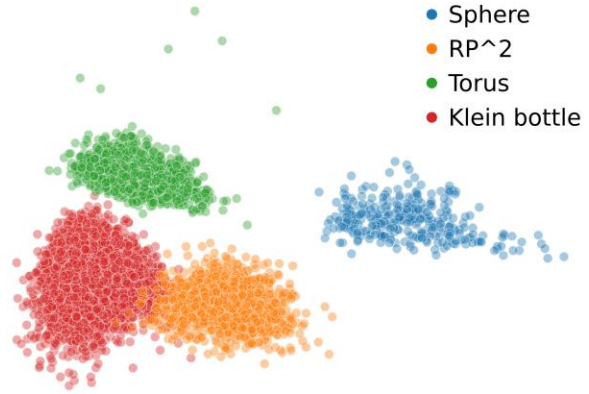
distinguish single-cell graphs




characterise molecular graph datasets

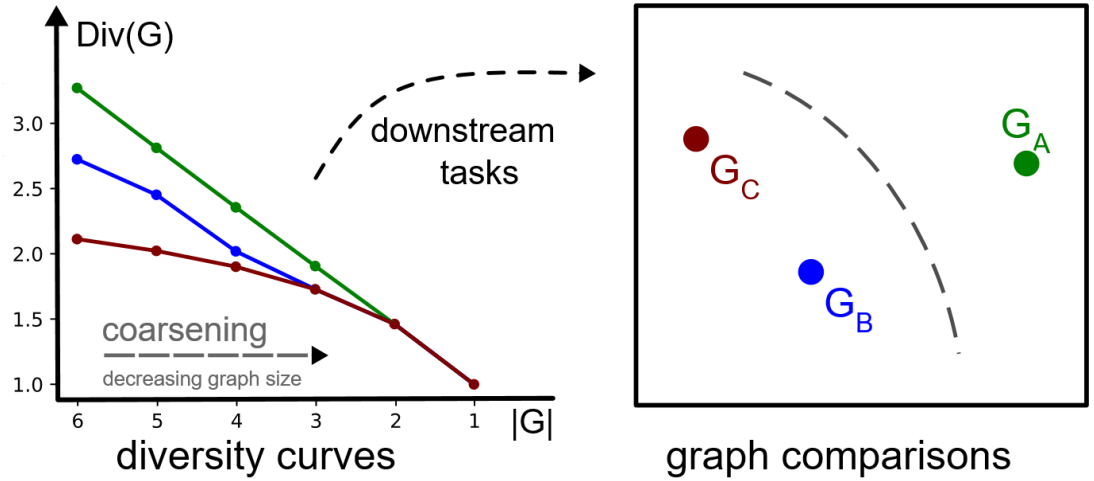



encode geometric shapes



# Diversity curves as graph representation

We propose diversity curves, novel **graph-level representations** for unsupervised tasks that **track structural diversity across coarsening levels**.




Paper

Code