# Strengthening structural baselines for graph classification using Local Topological Profile

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# Graph classification

- **task:** assign a label to a whole graph
- **examples:**
  - molecules, e.g. mutagenicity, toxicity
  - proteins, e.g. enzyme or not
  - social networks, e.g. type of community

# Main approaches

**Feature extraction:**

- extract features from the graph into a tabular form
- classify with any classic algorithm
- often called **graph embedding**
- simple, but very fast and scalable

# Main approaches

**Graph kernels:**

- direct all-pairs similarity comparison
- costly and the least scalable

# Main approaches

**Graph Neural Networks (GNNs):**

- learnable, task-specific feature extraction
- the most modern approach
- use: topology, node features, edge features (sometimes)
- suffer from overfitting, oversmoothing, lack of data, training instability etc.
- nevertheless, often seem to give the best results

# Local Degree Profile (LDP)

- Cai, Chen, and Yusu Wang. "A simple yet effective baseline for non-attributed graph classification."
- **structural** (topological) feature extraction method
- designed as a **baseline** method for graph kernels and GNNs, widely used
- **idea:**
  - extract 5 degree features for each node
  - aggregate with histograms (or EDF)
  - classify with kernel SVM

# LDP - details

- **LDP features:**
  - node degree, neighbors degrees statistics: min, max, mean, stddev
- **hyperparameters:**
  - number of bins
  - aggregation: histogram vs EDF
  - degree normalization: per graph vs per dataset
  - use log scale or not

# LDP - problems

- **strictly local:** degree is a strictly local descriptor
- **not scalable:** kernel SVM is not scalable, and requires hyperparameter tuning
- **sequential:** both for feature extraction (NetworkX) and for training (SVM + grid search)
- **many hyperparameters:** too many for a simple baseline
- **worrying methodology:** authors report validation set accuracy

# Solution: LTP

- we analyzed all 5 areas, and **improved all of them**
- our resulting method is **Local Topological Profile (LTP)**
- an iterative improvement, being:
  - 2-3 degrees of magnitude faster
  - better results
  - more scalable

# Local Topological Profile (LTP)

- **more global:** add 3 new, well selected descriptors
- **scalable:** uses Random Forest (RF)
- **parallel:** both for feature extraction (torch-scatter, NetworKit) and for training
- **no hyperparameters:** we show that none are necessary
- **fair methodology:** we use fair comparison procedure for GNNs from:

Errica, Federico, et al. "A fair comparison of graph neural networks for graph classification."

# LTP - additional descriptors

- **edge betweenness centrality** - measures edge importance:

$$EBC(e) = \sum_{s,t;(s,t)\neq(u,v)} \frac{\sigma_{st}(e)}{\sigma_{st}}$$

- **Jaccard index** - measures node clustering structure:

$$JI(u,v) = \frac{|N(u) \cap N(v)|}{|N(u) \cup N(v)|}$$

- **Local Degree Score** - measures "hubness" of nodes:

$$LDS(e) = \max\left(1 - \frac{\ln \operatorname{rank}(v,u)}{\ln \operatorname{degree}(v)}, 1 - \frac{\ln \operatorname{rank}(u,v)}{\ln \operatorname{degree}(u)}\right)$$

# LTP - Random Forest

- Random Forests are fast and **embarassingly parallel**, which makes them much more scalable than SVM
- they are **not sensitive to hyperparameter choice**, so we can omit tuning
- they consider each feature individually - we can **eliminate 2 hyperparameters:** aggregation and normalization

# LTP - hyperparameters

- we experimentally verify that we can set **reasonable defaults** for number of bins, and that we do not need log scale
- combined with RF, this **eliminates all hyperparameters**, with no (or negligible) decrease in accuracy

# LTP - parallelization

- LDP used sequential, Python-based NetworkX for feature extraction
- computing our new features **may be** costly
- we use parallel libraries torch-scatter and NetworKit, written in C++
- this improvement alone **completely offsets**, by a large margin, the added cost

# LTP - methodology

- we use **nested cross-validation** for evaluation:
  - 10-fold CV for testing
  - 5-fold CV for validation
- as described in fair comparison procedure for GNNs we use exactly the same folds as that paper
- we report results both for LDP and for our proposed LTP under this methodology
- benchmark is a standardized collection of 9 reasonably large graph classification datasets

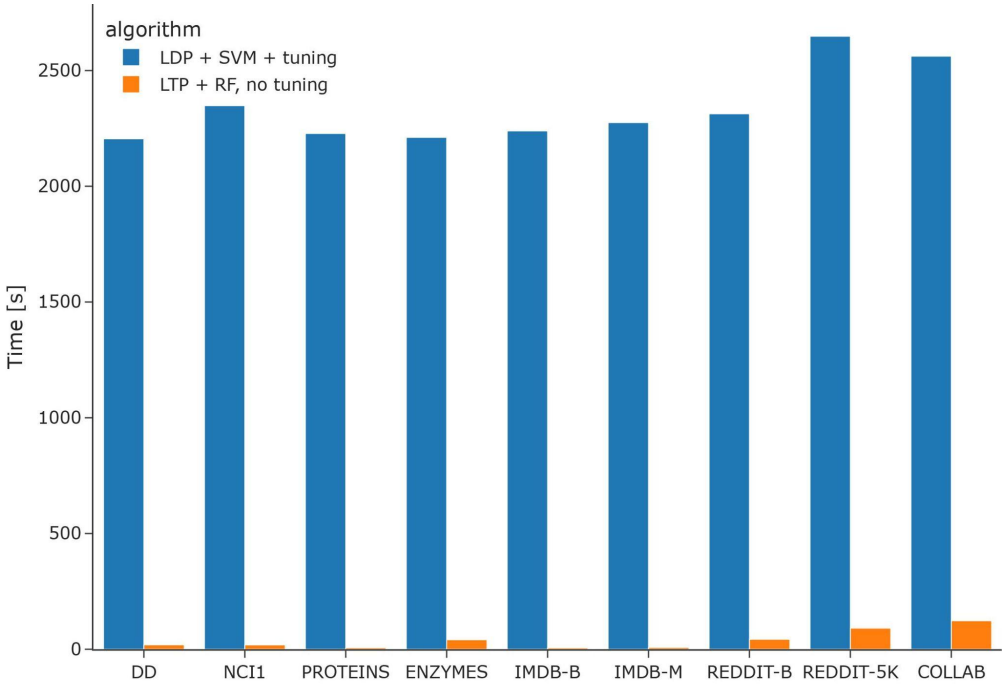
# Datasets

| Dataset | # Graphs | Avg. # Nodes | Avg. # Edges | # Classes |
|---|---|---|---|---|
| DD | 1178 | 284.32 | 715.66 | 2 |
| NCI1 | 4110 | 29.87 | 32.30 | 2 |
| PROTEINS | 1113 | 39.06 | 72.82 | 2 |
| ENZYMES | 600 | 32.63 | 64.14 | 6 |
| IMDB-B | 1000 | 19.77 | 96.53 | 2 |
| IMDB-M | 1500 | 13.00 | 65.94 | 3 |
| REDDIT-B | 2000 | 429.63 | 497.75 | 2 |
| REDDIT-5K | 4999 | 508.82 | 594.87 | 5 |
| COLLAB | 5000 | 74.49 | 2457.78 | 3 |

# Results - scalability

**Note:** we re-implemented LDP with torch-scatter and used parallel grid search.

With original implementation, LDP would be at least 10-100x slower.



# Results - accuracy

| Dataset | Baseline [4] | DGCNN | DiffPool | ECC | GIN | GraphSAGE | LDP | LTP |
|---|---|---|---|---|---|---|---|---|
| DD | **78.4 ±4.5** | 76.6 ±4.3 | 75.0 ±3.5 | 72.6 ±4.1 | 75.3 ±2.9 | 72.9 ±2.0 | 76.0 ±3.0 | 77.1 ±3.7 |
| NCI1 | 69.8 ±2.2 | 76.4 ±1.7 | 76.9 ±1.9 | 76.2 ±1.4 | **80.0 ±1.4** | 76.0 ±1.8 | 77.2 ±1.5 | 77.0 ± 1.9 |
| PROTEINS | **75.8 ±3.7** | 72.9 ±3.5 | 73.7 ±3.5 | 72.3 ±3.4 | 73.3 ±4.0 | 73.0 ±4.5 | 70.6 ±1.7 | 72.7 ±4.2 |
| ENZYMES | **65.2 ±6.4** | 38.9 ±5.7 | 59.5 ±5.6 | 29.5 ±8.2 | 59.6 ±4.5 | 58.2 ±6.0 | 37.4 ±4.0 | 42.5 ±4.1 |
| IMDB-B | 70.8 ±5.0 | 69.2 ±3.0 | 68.4 ±3.3 | 67.7 ±2.8 | 71.2 ±3.9 | 68.8 ±4.5 | 71.3 ±3.3 | **74.5 ±4.3** |
| IMDB-M | 49.1 ±3.5 | 45.6 ±3.4 | 45.6 ±3.4 | 43.5 ±3.1 | 48.5 ±3.3 | 47.6 ±3.5 | 49.0 ±4.4 | **50.0 ±4.6** |
| REDDIT-B | 82.2 ±3.0 | 87.8 ±2.5 | 89.1 ±1.6 | OOR | 89.9 ±1.9 | 84.3 ±1.9 | 89.6 ±1.2 | **91.1 ±1.0** |
| REDDIT-5K | 52.2 ±1.5 | 49.2 ±1.2 | 53.8 ±1.4 | OOR | **56.1 ±1.7** | 50.0 ±1.3 | 51.9 ±1.6 | 53.3 ±1.5 |
| COLLAB | 70.2 ±1.5 | 71.2 ±1.9 | 68.9 ±2.0 | OOR | 75.6 ±2.3 | 73.9 ±1.7 | 75.7 ±2.0 | **79.4 ±2.5** |

# Results - model ranks

| | Baseline [4] | DGCNN | DiffPool | ECC | GIN | GraphSAGE | LDP | LTP |
|---|---|---|---|---|---|---|---|---|
| **Average rank** | 3.8 | 5.2 | 4.6 | 7.6 | 2.7 | 5.4 | 4 | **2.6** |

# Summary

- we analyze existing structural baseline, Local Degree Profile (LDP)
- based on results, we identified 5 areas for improvement
- we propose **Local Topological Profile (LTP)** as a strengthened structural baseline
- LTP has better scalability and accuracy
- it can even outperform modern GNNs

# Questions?