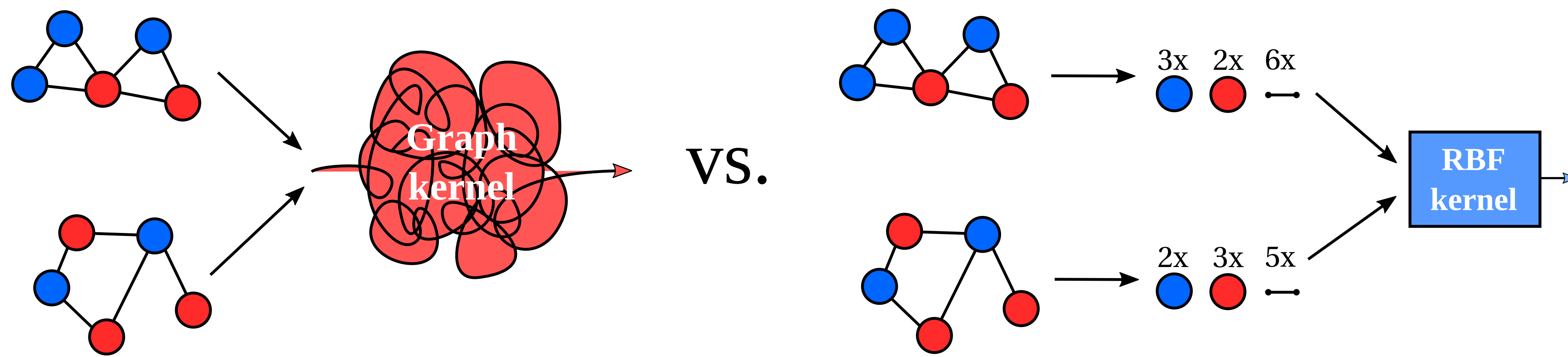


# On the Necessity of Graph Kernel Baselines

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## Is graph structure even relevant in classification tasks of benchmark datasets?

- We compare established graph kernels to a kernel which disregards *all* graph structure.
- The **No-Graph kernel (NoG)** considers graphs as a multiset of vertex and edge labels.



## How does NoG perform compared to more sophisticated graph kernels?

### Tested kernels:

- NoG - No-Graph baseline kernel
- psf - Probabilistic frequent subtree kernel [5]
- bpsf - Boosted probabilistic frequent subtree kernel [5]
- fsg - Frequent subgraph kernel based on FSG [7]
- cp - Cyclic pattern kernel [2]
- gs - Graphlet sampling kernel [4]
- sp - Shortest path kernel [1]
- rw - Random walk kernel [6]
- wl - Weisfeiler Lehman kernel [3]

### Evaluation details:

The predictive performance was measured in terms of accuracy obtained by SVMs using a 10-fold cross-validation. The kernel and SVM parameters were identified using an extensive grid search.

### Legend:

- no significant difference to NoG
- kernel performs significantly worse than NoG
- kernel performs significantly better than NoG
- x - result unavailable due to time/memory constraints

### Observations & Interpretations:

- No tested graph kernel achieves results significantly better than the baseline on more than a few datasets.
- Graph kernels can hardly prove their functionality on available datasets.
- Utilizing the graphs' structure in graph kernels does not significantly improve the classification accuracy.
- Graph structure may not even be relevant to perform well on a majority of benchmark datasets.

|                  | NoG   | psf   | bpsf  | fsg   | cp    | gs    | sp    | rw    | wl    |
|------------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| AIDS             | 99.65 | 98.25 | 98.45 | 97.85 | 98.60 |       |       |       | 98.70 |
| BZR              | 86.16 |       |       |       | 78.78 | 78.53 |       | 73.82 |       |
| BZR_MD           | 70.19 |       | 58.14 | x     | x     | 52.34 |       | 50.66 | 60.75 |
| COIL-DEL         | 14.13 | 7.83  | 7.68  | x     | x     | 9.74  |       | x     |       |
| COIL-RAG         | 7.22  | 3.38  | 3.36  | 5.69  | x     | 3.16  | 6.61  | x     |       |
| COX2             | 81.37 | 78.16 | 78.16 | 69.39 | 77.95 | 78.16 |       | 77.95 |       |
| COX2_MD          | 65.26 |       |       |       | x     | 51.81 |       | 51.15 |       |
| DD               | 76.67 |       |       |       | x     |       | x     | x     |       |
| DHFR             | 74.06 |       |       |       | 54.77 | 67.05 |       | 60.98 | 82.02 |
| DHFR_MD          | 64.88 |       |       | x     | x     |       | 69.20 |       |       |
| ENZYMES          | 43.33 | 28.33 | 32.00 | x     | x     | 30.50 |       | 17.33 | 50.67 |
| ER_MD            | 74.46 |       |       |       | x     | 59.42 | 59.21 | 59.42 |       |
| IMDB-BINARY      | 70.70 | 59.00 | 60.10 | 61.50 | x     | 63.90 | 47.90 | x     |       |
| IMDB-MULTI       | 46.73 | 38.93 | 40.13 |       | x     | 39.53 | 34.13 | x     |       |
| Letter-high      | 34.58 | 29.42 | 28.89 |       | x     | 18.70 | 30.47 |       |       |
| Letter-low       | 43.02 | 27.29 | 27.07 | 27.29 | x     | 14.93 | 48.60 | 47.04 | 39.91 |
| Letter-med       | 38.71 | 26.80 | 27.07 | 26.80 | x     | 14.51 | 44.67 |       |       |
| MSRC_21          | 86.46 | 51.84 | 52.22 | 46.79 | x     | 14.60 |       | 5.06  |       |
| MSRC_21C         | 81.59 |       |       | 64.63 | x     | 16.43 |       | 6.43  |       |
| MSRC_9           | 88.35 |       |       | x     | x     | 25.09 |       | 11.73 |       |
| MUTAG            | 87.31 |       |       |       |       |       |       |       |       |
| Mutagenicity     | 75.56 |       |       |       | 79.06 | 64.61 |       | x     | 83.56 |
| NCI1             | 69.93 |       | 74.33 | 76.28 |       | 62.68 |       | x     | 84.72 |
| NCI109           | 68.48 | 73.56 | 72.64 | 75.67 | 73.56 | 64.67 |       | x     | 85.20 |
| PROTEINS         | 74.58 |       |       | x     | x     |       |       | x     |       |
| PROTEINS_full    | 74.58 |       |       | x     | x     |       |       | x     |       |
| PTC_FM           | 63.63 | 58.17 |       |       |       | 57.08 | 57.85 |       |       |
| PTC_FR           | 67.25 |       |       |       |       | 65.53 |       | 65.25 |       |
| PTC_MM           | 66.70 |       |       |       | 61.93 | 61.31 |       | 61.62 |       |
| PTC_MR           | 57.60 |       |       |       |       |       |       |       |       |
| REDDIT-BINARY    | 83.50 | 55.75 | 57.70 | x     | x     | x     | x     | x     | 72.80 |
| REDDIT-MULTI-12K | 36.99 | 23.18 | 23.12 | x     | x     | x     | x     | x     |       |
| REDDIT-MULTI-5K  | 49.81 | 22.46 | 22.90 | x     | x     | x     | x     | x     |       |
| SYNTHETIC        | 50.00 |       |       | x     | x     |       |       |       |       |
| SYNTHETICnew     | 64.33 | 51.33 |       |       | x     |       |       | 54.00 | 99.33 |
| Synthie          | 50.69 |       | 42.28 | x     | x     | 41.32 |       | 16.05 |       |
| Tox21_AHR        | 90.89 | 88.47 | 88.36 | 88.37 |       | 88.38 | 88.41 | x     | 93.36 |
| Tox21_AR-LBD     | 98.05 |       |       |       | x     | 96.50 | 97.50 | x     | 98.49 |
| Tox21_ARE        | 86.42 | 84.79 | 84.74 | 84.69 | x     | 84.67 | 84.75 | x     | 88.94 |

## What do the results suggest?

- Most available datasets aren't suitable for benchmarking purposes.
- New benchmark datasets that highlight the power of graph kernels are necessary.
- Graph kernel baselines are imperative in order to put graph kernel performances into context.

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