
Erratum to "Scalable kernels for graphs with continuous attributes, NIPS 2013"

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It has come to our attention that there were errors in the experiments in the paper [1]. The errors affect our results on synthetic data, but the conclusions made in the paper still hold. We apologize deeply for any inconvenience caused by our mistakes.

The SYNTHETIC dataset. By mistake, all the graphs in the SYNTHETIC dataset used in [1] had the same graph structure. We have generated a synthetic dataset SYNTHETICnew as described in [1], and performed the classification experiments described in [1] on SYNTHETICnew. Results, along with the results on SYNTHETIC reported in [1], are found in Table 1. For the new SYNTHETIC dataset, the discrete Weisfeiler-Lehman kernel outperforms all other kernels. Other than that, the ranking of kernel performance is unchanged.

The ENZYMES dataset. The graphs in the ENZYMES dataset used in [1] were not symmetric. This is not an error per se, but in previously used versions of ENZYMES with discrete node attributes [2], these graphs were symmetrized. The WL kernel results reported in [1] were from the symmetrized version of the dataset.

To examine the effect of symmetrization, we perform classification experiments on a set ENZYMESsymm with symmetrized graphs, and compare to the results from [1], see Table 1. We find that symmetrization only appears to affect the performance of the PROP kernel.

The PROP kernels were by mistake ran on a version of ENZYMES whose node features had dimension 1, not 18. The results in Table 1 are for 18-dimensional features, giving lower PROP accuracy. This does not affect the conclusions made in [1].

Both the original datasets ENZYMES and SYNTHETIC, as well as the updated datasets ENZYMESsymm and SYNTHETICnew can now be downloaded from <http://image.diku.dk/aasa/software.php>.

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Kernel	ENZYMES	ENZYMESsymm	SYNTHETIC	SYNTHETICnew
GraphHopper	69.6 ± 1.3%	68.3 ± 0.9%	86.6 ± 1.0%	78.3 ± 1.5%
PROP-diff	21.9 ± 1.8%	17.7 ± 1.2%	46.1 ± 1.9%	51.4 ± 2.5%
PROP-WL	16.6 ± 1.1%	16.5 ± 1.2%	44.5 ± 1.2%	42.8 ± 2.4%
SP	71.0 ± 1.3%	72.3 ± 0.9%	85.4 ± 2.1%	82.5 ± 1.3%
CSM	69.4 ± 0.8%	69.5 ± 0.7%	–	–
WL	48.6 ± 1.0%	48.5 ± 0.7%	43.3 ± 2.3%	97.5 ± 2.4%

Table 1: Mean classification accuracies with standard deviation for all experiments, significantly best accuracies in bold. The CSM kernel did not finish within 30 days on the SYNTHETIC dataset, and was not ran on SYNTHETICnew (which has the same number of equally large graphs).

References

- [1] A. Feragen, N. Kasenburg, J. Petersen, M. de Bruijne, and K.M. Borgwardt. Scalable kernels for graphs with continuous attributes. In *NIPS*, pages 216–224, 2013.
- [2] N. Shervashidze, P. Schweitzer, E.J. van Leeuwen, K. Mehlhorn, and K.M. Borgwardt. Weisfeiler-Lehman graph kernels. *JMLR*, 12:2539–2561, 2011.