Supplementary Material
cblearn: Comparison-based Machine Learning in Python

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Empirical evaluation

We generated embeddings of comparison-based datasets to measure runtime and triplet error as a small empirical evaluation of our ordinal embedding implementations. We compared various CPU and GPU implementations in `cblearn` with third-party implementations in R (`loe` Terada and Luxburg 2014), and *MATLAB* (Maaten and Weinberger 2012). In contrast to synthetic benchmarks (e.g., Vankadara et al. 2021), we used the real-world datasets that can be accessed through *cblearn*, converted to triplets. The embeddings were arbitrarily chosen to be 2D. Every algorithm runs once per dataset on a compute node (8-core of Intel®Xeon ®Gold 6240; 96GB RAM; NVIDIA 2080ti); just a few runs did not yield results due to resource demanding implementations or bugs: our *FORTE* implementation exceeded the memory limit on the *imagenet-v2* dataset, the third-party implementation of *tSTE* timed out on *things* and *imagenet-v2* datasets. The third-party *SOE* implementation reached a limit on dataset size on *imagenet-v2*. Probably due to numerical issues, our *CKL-GPU* implementation did not crash but returned non-numerical values on the *musician* dataset.

The benchmarking scripts and results are publicly available in a separate repository[1].

Is there a "best" estimator?

Comparing all ordinal embedding estimators in `cblearn`, *SOE*, *CKL*, *GNMDS*, and *tSTE* were performing about equally well in both runtime and accuracy (Figure 1). The GPU implementations are slower on the tested datasets and for *SOE* and *GNMDS* noticeably less accurate.

[1] https://github.com/cblearn/cblearn-benchmark

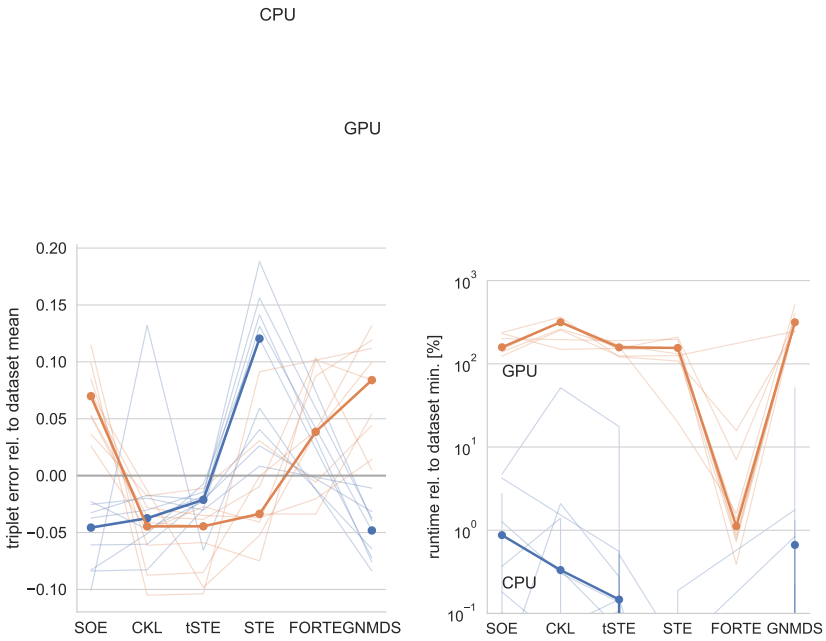


Figure 1: The triplet error and runtime per estimator, relative to the overall performance on the respective datasets. A smaller error indicates that more triplets of the dataset could be represented accurately in the 2D embedding. Grey lines show individual runs on the different datasets; the colored lines indicate the respective median performance.

When should GPU implementations be preferred?

In terms of accuracy and runtime, our GPU (or `pytorch`) implementations could not outperform the CPU (or `scipy`) pendants on the tested datasets. However, Figure 1 shows the GPU runtime grows slower with the number of triplets, such that they potentially outperform CPU implementations with large datasets of 10^7 triplets and more. In some cases, the GPU implementations show the overall best accuracy. An additional advantage of GPU implementations is that they require no explicit gradient definition, which simplifies the implementation of new algorithms.

There are various explanations for the speed disadvantage of our pytorch implementations. On the one hand, it may be due to the overhead of converting between numpy and pytorch and calculating the gradient (AutoGrad). On the other hand, it can also be due to the optimizer or the selected hyperparameters. To get a first impression of these factors, we have built a toy example, linear regression with 200 observations and 100 dimensions. The Figure 3 shows that the overhead of autograd and the stochastic optimization (Adam, lr=0.05) both

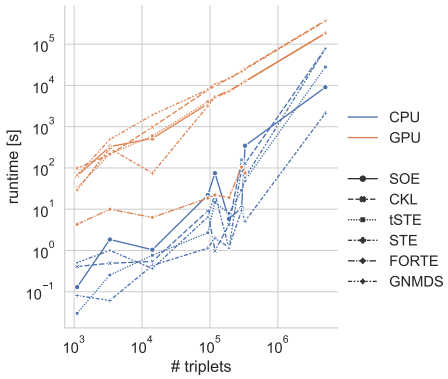


Figure 2: The runtime increases almost linearly with the number of triplets. However, GPU implementations have a flatter slope and thus can compensate for the initial time overhead on large datasets.

slow down the optimization multiplicatively by factor ~8 in this example. However, it can be assumed, and in accordance with the above tendency, that this disadvantage decreases with increasing data set size.

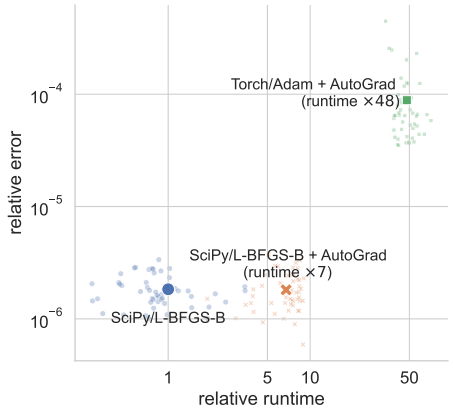


Figure 3: The runtime and error for different optimization methods in a toy example.

An additional disadvantage of stochastic optimizers like Adam is, that they are more sensitive to hyperparameter choices and thus require more tuning. This sensitivity is demonstrated in Figure 4, where the learning rate of Adam is varied for the toy example. Especially runtime largely depends on the learning rate, while the error is less sensitive to it. Likewise, the performance of `pytorch` ordinal embedding implementations could be improved by using more sophisticated tuning of optimizer parameters.

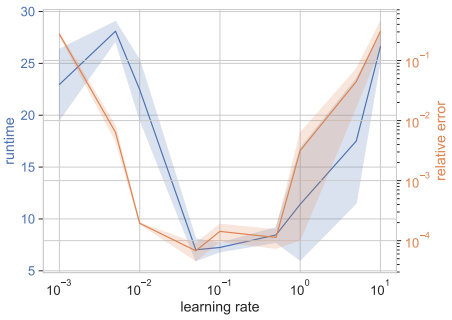


Figure 4: The runtime and error for different learning rates of the Adam optimizer in a toy example.

How does `cblearn` compare to other implementations?

In a small comparison, our implementations were $50 - 100\%$ faster with approximately the same accuracy as reference implementations (Figure 5). We compared our CPU implementations of *SOE*, *STE* and *tSTE* with the corresponding reference implementations in R , `loe` (Terada and Luxburg 2014), and *MATLAB* (Maaten and Weinberger 2012). Additionally, the latter offers an *CKL* implementation to compare with. Please note that despite our care, runtime comparisons of different interpreters offer room for some confounding effects. The results shown should nevertheless indicate a trend.

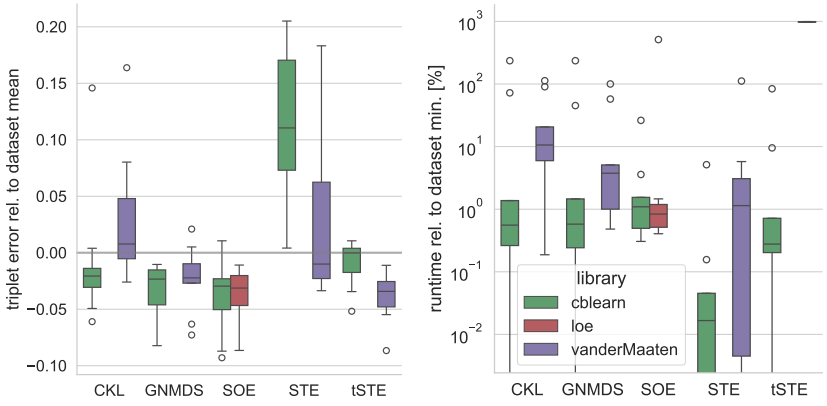
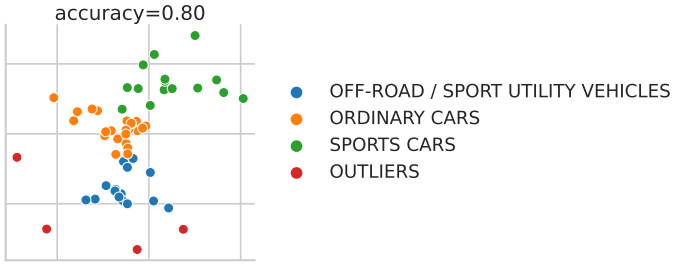


Figure 5: The triplet error and runtime improvement per estimator. Improvement is calculated against the average performance per dataset of all estimators in the plot.

Code example

```
from cblearn import datasets, preprocessing, embedding
from sklearn.model_selection import cross_val_score
import seaborn as sns; sns.set_theme("poster", "whitegrid")

cars = datasets.fetch_car_similarity()
triplets = preprocessing.triplets_from_mostcentral(cars.triplet, cars.response)
accuracy = cross_val_score(embedding.SOE(n_components=2), triplets, cv=5).mean()
embedding = embedding.SOE(n_components=2).fit_transform(triplets)
fg = sns.relplot(x=embedding[:, 0], y=embedding[:, 1],
        hue=cars.class_name[cars.class_id])
fg.set(title=f"accuracy={accuracy:.2f}", xticklabels=[], yticklabels=[])
fg.tight_layout(); fg.savefig("images/car_example.pdf")
```



References

Maaten, Laurens van der, and Kilian Weinberger. 2012. "Stochastic Triplet Embedding." In *International Workshop on Machine Learning for Signal Processing*, 1–6. https://doi.org/10.1109/MLSP.2012.6349720.

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Vankadara, Leena Chennuru, Siavash Haghiri, Michael Lohaus, Faiz Ul Wahab, and Ulrike von Luxburg. 2021. "Insights into Ordinal Embedding Algorithms: A Systematic Evaluation." *arXiv:1912.01666 [Cs, Stat]*. https://doi.org/10.48550/arXiv.1912.01666.