





















measure of performance, this should convincingly indicate that the top- $k$  criterion is fundamentally inferior to the max- $k$  criterion.

This is further confirmed by comparing the F1 score of the sampling and greedy protocols against that of the **TopK\_Oracle** limit. The F1 performances of all four models under these two protocols exceed **TopK\_Oracle**, the theoretical upper limit that all possible models can ever achieve under the top- $k$  criterion.

Besides, when applying the TopK protocol on the model's predictive distribution, we see that its F1 score is only slightly lower than the **TopK\_Oracle** F1 curve and the gap between the two curves diminishes with  $k$ . That is, with the top- $k$  criterion, there is little need to further improve the model, particularly at large  $k$ .

**6.2.5 Comparing Models and Datasets Under The Max-K Criterion.** Using a similar approach as that in Section 6.2.4, we now compare three state-of-the-art models, ComplEx, Analogy and ProjE, and assess the datasets with respect to these models.

The plots in Figure 4 are in the same form as those in Figure 3, except that we here only include the F1 metric. From the figure, one can conclude that under the F1 metric, ComplEx and Analog behave nearly identically. On FB15K, WN18 and WN18RR, they both outperform ProjE by a visible margin. On YAGO3-10, the three models have very similar performance. For each of the examined dataset in Figure 4, when comparing the model performance against the **MaxK\_Oracle** limit, it is interesting to observe that on WN18, there is only very small gap between the **MaxK\_Oracle** curve and the curves of these state-of-the-art models. That is, on this dataset, the performance of the current state of the art has already approached the ultimate limit. As such, we believe that on the WN18 dataset, further improvement upon these models will be very difficult, hence anticipating little progress in the coming years.

However, on FB15K, YAGO3-10 and particularly on WN18RR, the performance of the three models is still far away from the **MaxK\_Oracle** limit. This suggests that there is still significant room for developing innovative models to further improve the performance on these datasets. One should not expect a model to achieve the **MaxK\_Oracle** limit. To what extent a model can approach the **MaxK\_Oracle** performance is in fact governed by the learnability bound (intrinsically dictated by the structure and size of the data), living somewhere below the **MaxK\_Oracle** curve.

## 7 CONCLUDING REMARKS

Although the context of this work is link prediction in KBs, the max- $k$  criterion and the protocols introduced in this paper in general apply widely to information retrieval, multi-label classification and many related areas. This criterion is practically motivated and at the same time theoretically sound. The proposed sampling and greedy protocols also have a theoretical foundation and a universal applicability. We anticipate that the max- $k$  criterion and the proposed protocols find many applications beyond link prediction in KBs. Return to this context, we suggest that the conventional metrics used for link prediction be discarded, and replaced by the precision, recall and F1 metrics introduced herein.

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