

# Improving Extrapolation in Ranking Tasks

Extrapolation remains a challenge for machine learning models, particularly in areas such as drug design and materials science. In these fields, accurate ranking of outliers is crucial.

## Problem

How can we improve the accuracy of ranking high-performing samples that fall outside the training data range?

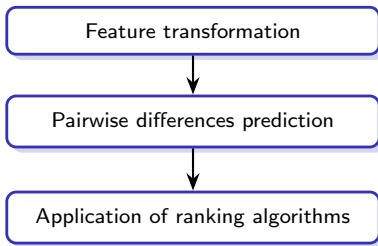
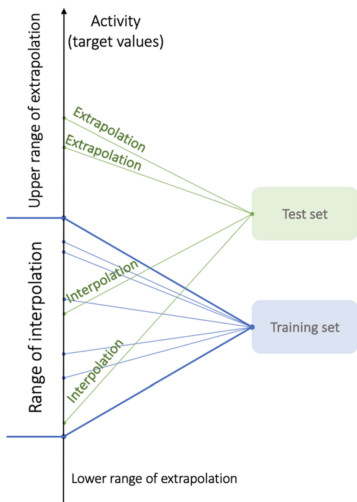
## Method

Using a pairwise learning approach: instead of predicting absolute target values, we predict the relative differences between samples, which are then processed by ranking algorithms.

## Contribution

Proposed method enhances extrapolation ability, improving model performance in ranking and identifying high-performing samples that exceed the training data.

# Pairwise Learning Approach



## Key metrics

- ▶  $f1_{top10}$  — F1 score of a ML method to retrieve top 10% samples.
- ▶  $f1_{extrap}$  — F1 score of a ML method to retrieve extrapolating samples.