The effect of pipeline-collection-diversity on performance

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August 31, 2020

Abstract

Do performers who submit diverse collections of pipelines tend to perform better than those who submit less diverse collections of pipelines? The answer for the Winter 2020 evaluation is effectively no. While there does exist statistically significant effect of increased diversity on increased score, the effect size is trivial. Thus, it seems that less diverse collections of pipelines, i.e. those that focus more on hyperparameter tuning, can as effective (or almost as effective, on average) as those that explore a greater diversity and/or ordering of primitives.

1 Introduction

In section 2, Measures of Diversity, we define several measures of the diversity within a collection of three or more pipelines. In section 3, Results at a Glance, we present a heat map showing briefly the (weak) connection between diversity and performance. In section 4, Quantifying the Effect of Diversity, we report on regression results which point to the measurable, though substantively trivial, effect of diversity on score. In a final section 5, Visualizing Collections we show a visualization of collections of pipelines for a problem together with a multiple alignment, for context.

2 Measures of Diversity

Before we can define diversity of a collection of (say 3 to 20) pipelines, we first need to define the distance between a pair of pipelines. We choose the Levenshtein edit distance as this measure between two pipelines. Specifically, we first express the pipelines as sequences of primitives, where primitives are written as "letters" in a large alphabet. The software we use accommodates all D3M primitives with two-letter pairs, each pair representing a single token (primitive) of the alphabet. The Levenshtein edit distance is the minimum number of substitutions, insertions and/or deletions needed to bring one sequence to coincide with the other. This measure satisfies the axioms for a distance.

But distance involves just two pipelines; diversity measures variation among a collection of three or more pipelines. We tried several alternatives for quantifying diversity. The most well-behaved measures (i.e. the ones that behave most closely to our expectations on synthetic data) were vector norms where the vector components were the Levenshtein distances for all possible unordered pairs of pipelines in the collection.

More precisely, we used l_p norms where p was a parameter varying between 1 and ∞ . The different norms measure slightly different quantities. At the extreme, the l_{∞} norm (maximum edit-distance component) is large when there is at least one pair of pipelines at great distance, regardless of the positions (great or small) of the other as-close or closer distances. On the other hand, the l_1 norm (sum of the edit-distance components) can still be relatively large if there are many pairs pipelines at moderate distance, even though there is no pair at great distance. We point out that the choice the different norms can sometimes matter: we have noted that the choice can order sets of collections—synthetic or real—differently in terms of diversity.

In the l_p norm, what value for the parameter p do we pick? If you are using only one measure of diversity, we recommend the l_2 norm as a nice trade off between the two extremes. That said, it is more informative to report two or more measures of diversity, in which case l_1 and l_{∞} should be preferred because they are most independent.

3 Results at a Glance

Figure 1 shows the diversity of performer pipeline submissions by problem type. The color-coding indicates diversity, with purple colors indicating small l_2 edit distance norms, trending towards yellow colors indicating larger l_2 edit distance norms. The number of asterisks in each cell captures the count of times a pipeline in that performer-category was the best (or tied). For instance, in the second row of the first column, UCB twice had the best-performing pipeline on a data set in the binary_classification problem category. Overall, the figure suggests (and we quantify below) a very small but measurable effect of diversity.

4 Quantifying the Effect of Diversity

We use regression-based methods to quantify the effect of diversity on performance. We address complications by combining several overlapping methodologies. Overall, our goal is to specify predictive models of performance. Our unit of analysis is a collection of pipelines submitted by a performer for a particular problem. The response variable is the best score of all pipelines in the collection. Our models predict best score based on three explanatory variables: the l_1 and l_{∞} norms for the collection (as discussed above), as well as "count," the number of pipelines in the collection.

The fact that different metrics were used for scoring different problems forced us to make adjustments. In some cases the best score was the greatest score, whereas in others the best score was the least score. By reversing the sign where appropriate, we transform scores so that greatest score was always best score. Our response variable was then called "max_score."

The fact that max_scores were on widely different scales across problems forced us to switch to standardized coordinates (z-scores) for max_score. The population for this standardization was all collections for all performers for one particular problem—as these were guaranteed to have metrics on the same scale.

At this point, we also transformed the predictor variables to standardized coordinates (against the same population), making predictors comparable only to other predictors for that problem.

Below, we report on five classes (A-E) of statistical models. For the purposes of analysis, we grouped problems by eleven categories (e.g. time series, binary classification, etc). See the horizontal axis of Figure 1 for a list of our categories.

In the first model, we group all problem categories together for analysis in a "complete pooling" model; see MODEL A.

In the second, we ran a fixed effects model (MODEL B) on category.

Third, we then ran a no pooling model (MODEL C), which is actually numerous separate models, one for each category.

We then ran a hierarchical model with random effects on the intercept (MODEL D).

Finally, we ran a hierarchical model with random effects on both the intercept and slope (MODEL E).

In all models, we see that there is a significant effect of l_1 z-score diversity on performance, but the coefficient is small (less than .2). The fact that we are using z-scores for both the predictors and response variable complicates the interpretation of this result. What it says is that for an increase of z-score of the predictor variable (l_1 z-score) by 1 the model predicts that the response variable (max_score z-score) will increase by almost 0.2. Put another way when the raw l_1 increases by one standard deviation for that problem, max_score increases by almost 0.2 standard deviations for that problem.

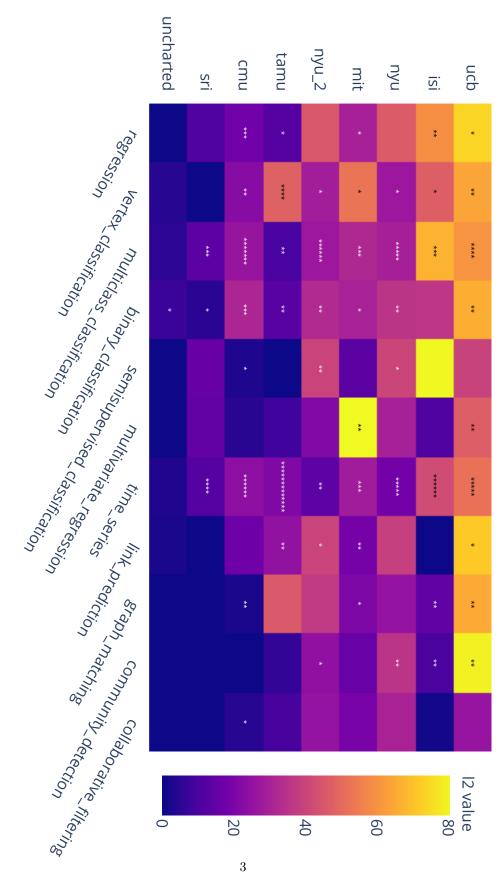
It is helpful to translate this result into raw scores for l_1 . A unit increase in l_1 means an one extra substitution, insertion, or deletion is needed to bring just one pair of pipelines to coincidence. We keep z-scores for max_score because raw scores for max_scores are meaningless for across-problem comparison. To convert to a transformation from a unit increase in raw l_1 to a specified z-score increase of max_score, we must divide the coefficient (about 0.2, depending on model) by the standard deviation of l_1 for the population referenced by the z-score. Of course, each problem has a different reference population so each problem has a different standard deviation. By implication, the transformed slopes will be different for each problem, but we can obtain summaries of the distribution of these slopes.

The 5-number summary of this distribution of slopes is

[0.00037622, 0.00052519, 0.00067828, 0.00114945, 0.00809511],

showing that a unit increase in l_1 leads to at most a 8-thousanths increase in the z-score of max_score, and the increase is usually quite a bit less. Our conclusion is that diversity has a negligibly small effect

Performer



to an additional 37 asterisks in the figure beyond the total number of 103 problems. The number of asterisks in each cell is the number of problem instances in the corresponding category-performer which was quantify diversity. The horizontal axis is the problem category and the vertical axis is performer for the Winter 2020 evaluation. the best (or tied for best) performing pipeline for any problem. There were 37 ties (including multi-way ties), corresponding Figure 1: Heat map of l_2 diversity see section "Measures of Diversity" for a discussion of this and other measures we use to

Category

Model	Coefficient	p-value	estimate	std error
A	l_1 (z-score)	0.00716 **	1.984e-01	7.355e-02
В	l_1 (z-score)	0.00763 **	1.984e-01	7.414e-02
\mathbf{C}	l_1 (z-score)	multiple models, same story.		
D	l_1 (z-score)	0.00716 **	1.984e-01	7.355e-02
\mathbf{E}	l_1 (z-score)	0.0155 *	1.778e-01	7.329e-02

Table 1: Summary of models predicting the z-score of a performer's best score in a submitted collection, based on l_1 and l_{∞} measures of diversity of the collection and count of number of pipelines in the collection. We performed a regression analysis with 5 different models (A-E, see text). The table shows the model, the coefficient examined (in this case, always considered just l_1 , among other predictors we used: l_{∞} and count). Furthermore, the table shows p-values (two tailed, under the null hypothesis that coefficient is zero), estimates of coefficients and standard errors of the estimates. Note that several entries of the table are identical to our numerical precision. We attribute this result to category-level predictors that do not covary with response variable. We examine the effect of colinearity between l_1 and l_{∞} and found that it did not change our results substantially. Significance codes: 0 "***" 0.001 "**" 0.05 "." 0.1 [blank] 1.

on performance.

Table 1 summarizes our results.

5 Visualizing Collections

In this final section, we show a cartoon visualization of collections of pipelines for a problem together with a multiple alignment (see Figure 2, and its caption).

See Following Pages

Figure 2: The next several pages show a cartoon figure of a multiple sequence alignment of all submitted pipelines (all performers) for one randomly selected problem semi_1217_click_prediction_small_MIN_METADATA. The circles in the first pane illustrate the pipelines and are referenced with the number that corresponds to the label in the multiple alignment in the second pane. The colors correspond to different performers (also labeled in the second pane). The alphabet used to label primitives is shown on the third pane, which was randomly generated. The position of the circles was determined by a spring layout procedure with pipelines close in edit distance supposedly remain close as nodes. That said, usually impossible solve this problem perfectly (at least in two dimensions) and we have noted that the software returns some misleading results while presumably trying to draw a pretty picture (what it was designed to do). Nevertheless, we found these figures useful for keeping pipelines in memory—as long as the image is interpreted as a "cartoon" and not a "topographical map." Cartoons for the other problems are available upon request.