## The effect of pipeline-collection-diversity on performance

## Sean Carver @ Data Machines Corporation

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 a 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 be 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  $\infty$ . The different norms measure slightly different quantities. At the extreme, the  $l_\infty$  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  $l_\infty$  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  $l_{\infty}$  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 on performance.

Table 1 summarizes our results.

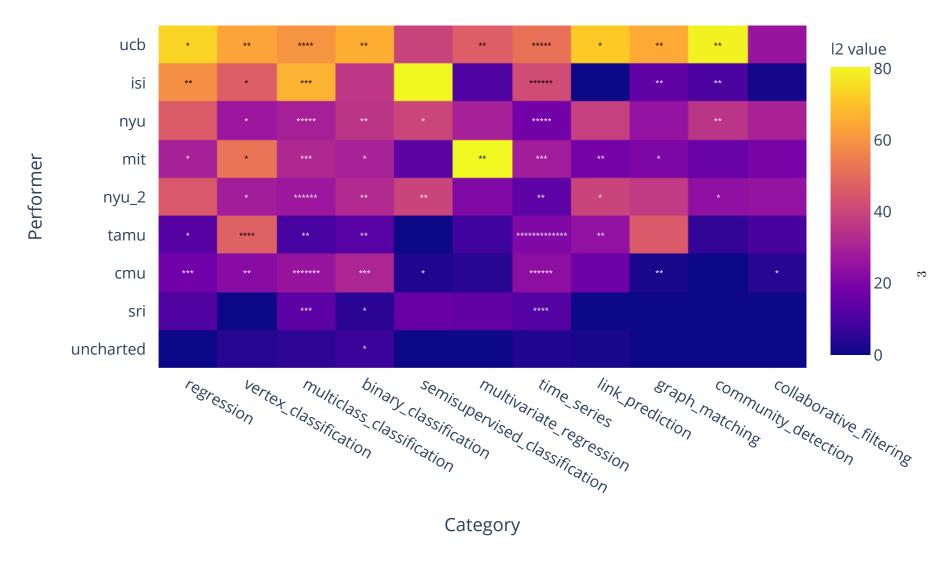


Figure 1: Heat map of  $l_2$  diversity see section "Measures of Diversity" for a discussion of this and other measures we use to quantify diversity. The horizontal axis is the problem category and the vertical axis is performer for the Winter 2020 evaluation. The number of asterisks in each cell is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

| 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 |

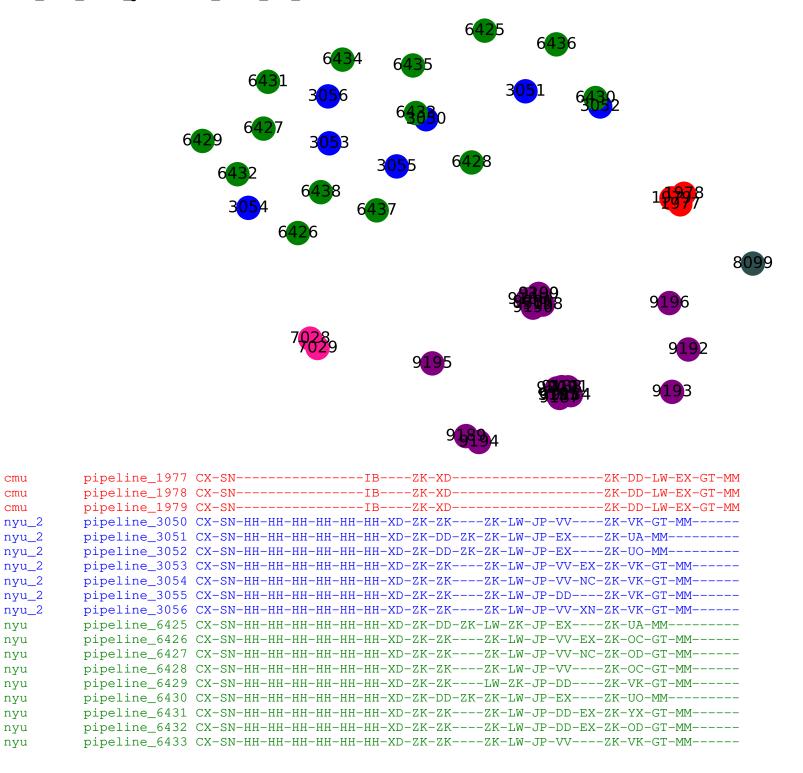
Table 1: Summary of models predicting the z-score of a performer's best score in a submitted collection, based on  $l_1$  and  $l_{\infty}$  measures of diversity of the collection and count of number of pipelines in the collection. We performed a regression analysis with 5 different models (A-E, see text). The table shows the model, the coefficient examined (in this case, always considered just  $l_1$ , among other predictors we used:  $l_{\infty}$  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  $l_{\infty}$  and found that it did not change our results substantially. Significance codes: 0 "\*\*\*" 0.01 "\*\*" 0.05 "." 0.1 [blank] 1.

## 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.



#### SEMI\_1217\_click\_prediction\_small\_MIN\_METADATA

| nyu       | pipeline_6434 | СХ-SN-НН-НН-НН-НН-НН- | -HH-XD-ZK-ZK     | -ZK-LW-JP-DD-EX- | -ZK-VK-GT-MM       |
|-----------|---------------|-----------------------|------------------|------------------|--------------------|
| nyu       | pipeline_6435 | CX-SN-HH-HH-HH-HH-HH- | -HH-XD-ZK-ZK     | ZK-LW-JP-VV      | -ZK-OD-GT-MM       |
| nyu       | pipeline_6436 | CX-SN-HH-HH-HH-HH-HH- | -HH-XD-ZK-ZK-LW- | ZK-ZK-JP-DD      | UM-GT-MM           |
| nyu       | pipeline_6437 | CX-SN-HH-HH-HH-HH-HH- | -HH-XD-ZK-ZK     | ZK-LW-JP-DD      | -ZK-YC-GT-MM       |
| nyu       | pipeline_6438 | CX-SN-HH-HH-HH-HH-HH- | -HH-XD-ZK-ZK     | ZK-LW-JP-DD      | -ZK-TX-GT-MM       |
| uncharted | pipeline_7028 | CX-SN                 | -BD-XD-DD-RT     |                  | -ZK-ZK-XH-MM       |
| uncharted | pipeline_7029 | CX-SN                 | -BD-XD-DD-RT     |                  | -ZK-ZK-XH-MM       |
| tamu      | pipeline_8099 | SN                    | -IB-XD-ZK-ZK     |                  | -DD-JO-GT-MM       |
| sri       | pipeline_9184 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9185 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9186 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9187 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9188 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9189 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-LW-JA-MM |
| sri       | pipeline_9190 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9191 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9192 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-XJ-WE-MM |
| sri       | pipeline_9193 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-LW-WE-MM |
| sri       | pipeline_9194 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-LW-JA-MM |
| sri       | pipeline_9195 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-AG-MM    |
| sri       | pipeline_9196 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-OD-IP-MM |
| sri       | pipeline_9197 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
| sri       | pipeline_9198 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9199 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9200 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9201 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-IP-MM    |
| sri       | pipeline_9202 | NI-SN                 | -IB-XD-ZK-KG     |                  | -ZK-GT-UG-WE-MM    |
|           |               |                       |                  |                  |                    |

```
AB: Multi Table Deep Feature Synthesis
AG: sklearn.ensemble.bagging.BaggingClassifier
AO: OWLRegression
AQ: jhu.gclust
AW: sklearn.decomposition.fastica_.FastICA
AX: sklearn.preprocessing.data.StandardScaler
BB: CorexContinuous
BD: simon
BH: sklearn.neural_network.multilayer_perceptron.MLPClassifier
BL: Columns text reader
BN: SDNE
BO: Annotated tabular extractor
BP: DeepAR
BU: Gaussian Latent Dirichlet Allocation Topic Modelling
CI: sklearn.linear_model.passive_aggressive.PassiveAggressiveClassifier
CK: sklearn.impute.SimpleImputer
CL: sklearn.svm.classes.SVR
CM: DSBox Unary Data Encoder
CR: sklearn.tree.tree.DecisionTreeClassifier
CS: sklearn.preprocessing._encoders.OrdinalEncoder
CT: find projections
CV: sklearn.ensemble.forest.RandomForestRegressor
CX: Denormalize datasets
DA: gator
DD: sklearn.impute.SimpleImputer
DE: sklearn.kernel_ridge.KernelRidge
DG: DSBox Image Featurizer VGG16
DI: sklearn.linear_model.base.LinearRegression
DL: STMBplus_auto feature selector
DN: jhu.link_pred_rc
DP: kanine
DR: Random forest classifier
DT: Random Sampling Imputer
DX: sklearn.linear_model.coordinate_descent.ElasticNet
DZ: Dataset Metafeature Extraction
EA: tsne
EH: Randomized Principal Component Analysis using Polynomial Features
EO: XGBoost GBTree classifier
EP: Binary encoder
ES: Extracts columns by structural type
EW: lupi_svm.LupiSvmClassifier
EX: sklearn.preprocessing.data.RobustScaler
EY: K means
FD: DSBox ensemble voting
FM: Label encoder with an unseen category
FN: DSBox Profiler
FP: ISI DSBox To Numeric DataFrame
FT: LightGBM GBTree classifier
FU: sklearn.svm.classes.LinearSVR
FX: sklearn.kernel_approximation.RBFSampler
GD: sklearn.svm.classes.SVC
GP: DSBox horizontal concat
GS: DataFrame to ndarray converter
GT: Iterative labeling for semi-supervised learning
HA: DSBox feature scaler
HC: jhu.ase
HG: ndarray to Dataframe converter
HH: Add semantic types to columns
HJ: sklearn.linear_model.bayes.ARDRegression
HL: Tensor Machine Regularized Least Squares
HM: Removes columns
HN: jhu.link_pred_graph_reader
HQ: DSBox vertically concat
HR: lupi_mfa.lupi_mfa.LupiMFA
```

HW: sklearn.random\_projection.SparseRandomProjection

```
IA: sklearn.ensemble.forest.RandomTreesEmbedding
IB: Determine missing semantic types for columns automatically
IH: Load single graph and dataframe into a parseable object
IM: DSBox Splitter
IP: sklearn.ensemble.gradient_boosting.GradientBoostingClassifier
IQ: sklearn.dummy.DummyClassifier
IR: sklearn.discriminant_analysis.LinearDiscriminantAnalysis
IS: ISI DSBox Data Encoder
IT: DSBox random projection timeseries featurization
JA: sklearn.neighbors.nearest_centroid.NearestCentroid
JH: CommunityDetection
JK: Enrich dates
JM: sklearn.gaussian_process.gpr.GaussianProcessRegressor
JN: EchoLinearRegression
JO: Text encoder
JP: Concatenate multiple dataframes
JW: sklearn.linear_model.stochastic_gradient.SGDRegressor
KA: sklearn.dummy.DummyRegressor
KF: Gaussian Mixture Models
KG: Autoflow Data Conditioner
KL: sklearn.discriminant_analysis.QuadraticDiscriminantAnalysis
KR: sklearn.ensemble.forest.ExtraTreesRegressor
KS: retina_net
KV: Map DataFrame resources to new resources using provided primitive
KW: sklearn.preprocessing.data.MaxAbsScaler
LB: XGBoost GBTree regressor
LC: Replace semantic types for columns
LF: Hierarchical Dirichlet Process Topic Modelling
LI: Latent Dirichlet Allocation Topic Modelling
LL: sklearn.linear_model.ridge.Ridge
LM: Grouping Field Compose
LT: Text Classifier
LW: sklearn.preprocessing.data.OneHotEncoder
LY: DataFrame Sampling
MF: SeededGraphMatcher
ML: Data cleaning
MM: Construct pipeline predictions output
MP: K-means Clustering
MU: sklearn.decomposition.truncated_svd.TruncatedSVD
MV: sklearn.random_projection.GaussianRandomProjection
MY: Nearest Neighbor Classification with Cover Trees
NA: find projections
```

NC: Regex dataset filter

ND: Nearest Neighbor Regressor with Cover Trees NF: Label decoder for UnseenLabelEncoderPrimitive

NG: DSBox Iterative Regression Imputer

NI: Columns text reader

NK: General Relational Dataset

NP: Image Transfer

NT: sklearn.preprocessing.data.MinMaxScaler

NU: RFM Preconditioned Polynomial Kernel Ridge Regression

NY: sklearn.naive\_bayes.GaussianNB

OB: sklearn.linear\_model.coordinate\_descent.LassoCV

OC: sklearn.feature\_selection.variance\_threshold.VarianceThreshold

OD: sklearn.feature\_selection.univariate\_selection.SelectPercentile

00: DSBox Arima Primitive

OP: CorexText

OQ: sklearn.ensemble.weight\_boosting.AdaBoostClassifier

PA: Columns image reader

PC: sklearn.feature\_selection.univariate\_selection.GenericUnivariateSelect

PE: jhu.gclass

PK: sklearn.ensemble.forest.ExtraTreesClassifier

PN: sklearn.ensemble.weight\_boosting.AdaBoostRegressor

PS: Huber PCA

PY: sklearn.linear\_model.least\_angle.Lars

- QM: sklearn.impute.MissingIndicator
- QN: Preprocessing for categorical columns
- QO: Extracts columns
- QQ: DSBox Timeseries Featurizer dataframe to List Transformer
- QT: RF Features
- QU: RFM Preconditioned Gaussian Kernel Ridge Regression
- RC: sklearn.linear\_model.stochastic\_gradient.SGDClassifier
- RE: VAR
- RF: sklearn.tree.tree.DecisionTreeRegressor
- RL: lupi\_rf.LupiRFClassifier
- RN: Load audio collection from dataset into a single dataframe
- RQ: sklearn.naive\_bayes.MultinomialNB
- RS: Single Table Deep Feature Synthesis
- RT: hdbscan
- SB: sklearn.neighbors.regression.KNeighborsRegressor
- SC: sklearn.ensemble.bagging.BaggingRegressor
- SD: DSBox Object Detection YOLO
- SK: List encoder
- SN: Extract a DataFrame from a Dataset
- SP: Robust Sparse Principal Component Analysis
- SR: Time series formatter
- ST: sklearn.feature\_extraction.text.CountVectorizer
- SU: Sparse Principal Component Analysis
- SW: Select dataframe from list of dataframes
- SY: DSBox Image Featurizer ResNet50
- TA: BERT pair classification
- TD: Audio Transfer
- TE: 1stm fcn
- TH: sklearn.cluster.hierarchical.FeatureAgglomeration
- TK: DSBox Cleaning Featurizer
- TL: find projections numeric
- TN: Dataset sampling primitive
- TV: DSBox Greedy Imputer
- TW: sklearn.decomposition.kernel\_pca.KernelPCA
- TX: JMIplus\_auto feature selector
- UA: sklearn.ensemble.forest.RandomForestClassifier
- UD: Remove semantic types from columns
- UG: Parses strings into their types
- UI: sent2vec\_wrapper
- UJ: Tree-Augmented Naive Bayes Classifier
- UL: find projections
- UM: sklearn.feature\_selection.univariate\_selection.SelectFwe
- UN: DSBox do-nothing primitive
- UO: sklearn.neighbors.classification.KNeighborsClassifier
- UR: sklearn.decomposition.pca.PCA
- UV: sklearn.linear\_model.coordinate\_descent.Lasso
- UX: Categorical imputer
- UY: Replace singeltons
- UZ: VertexNomination
- VB: LinkPrediction
- VH: Random Classifier
- VK: PCA Features
- VO: tsne
- VP: DSBox Image Featurizer dataframe to tensor transformer
- VS: Casts DataFrame
- VT: Load graphs into a parseable object
- VV: DSBox feature labeler
- VW: Collaborative filtering
- WA: jhu.sqm
- WB: Matrix Completion via Sparse Factorization
- WC: sklearn.neural\_network.multilayer\_perceptron.MLPRegressor
- WE: sklearn.naive\_bayes.BernoulliNB
- WI: Echo
- WJ: sklearn.preprocessing.data.QuantileTransformer
- WK: Extract a list of Graphs from a Dataset

- WR: sklearn.feature\_extraction.text.TfidfVectorizer
- WU: jhu.lcc
- WY: sklearn.linear\_model.passive\_aggressive.PassiveAggressiveRegressor
- WZ: Concatenate two dataframes
- XB: lupi\_rfsel.LupiRFSelClassifier
- XD: Parses strings into their types
- XH: EnsembleForest
- XI: Low Rank Imputer
- XJ: sklearn.preprocessing.data.PolynomialFeatures
- XK: sklearn.kernel\_approximation.Nystroem
- XN: sklearn.preprocessing.data.Binarizer
- XS: sklearn.ensemble.gradient\_boosting.GradientBoostingRegressor
- XT: One-hot encoder
- XV: Load edgelist into a parseable object
- XZ: sklearn.linear\_model.logistic.LogisticRegression
- YB: sklearn.preprocessing.data.Normalizer
- YC: S2TMBplus feature selector
- YJ: sklearn.svm.classes.LinearSVC
- YM: One-hot maker
- YN: jhu.lse
- YS: DSBox do-nothing primitive dataset version
- YX: Feature Selection
- ZB: XGBoost DART classifier
- ZF: DSBox Mean Imputer
- ZK: Extracts columns by semantic type
- ZR: Pandas one hot encoder
- ZZ: Perform dataset augmentation using Datamart