The effect of pipeline-collection-diversity on performance

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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.

Model	Coefficient	p-value	estimate	std error
A	l_1 (z-score)	0.00716 **	1.984e-01	7.355e-02
B	l_1 (z-score)	0.00763 **	1.984e-01	7.414e-02
C	l_1 (z-score)	multiple models, same story.		
D	l_1 (z-score)	0.00716 **	1.984e-01	7.355e-02
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 "**" 0.01 "*" 0.05 "." 0.1 *[blank]* 1.

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. This analysis is complicated by several factors, which we address by various, overlapping methodological choices. Overall, our goal is to specify predictive models of performance on the bases of the l_1 and l_∞ norms, as well as the number of pipelines submitted. Our unit of analysis is the collection of pipelines submitted by a performer, which features diversity measures mentioned, a count, and the score obtained by its best member. We group these by problem across performer for analysis. The diversity measures and scores are not comparable across problems, or problem types; thus, we move to measuring all predictors and scores on a per-problem z-score basis.

Below, we report on five classes of statistical models. In the first, we group all problem types together for analysis in a "complete pooling" model; see MODEL A.

First, ran a complete pooling model including fixed effects for problem type, and saw no change in our key predictors.

Second we ran a fixed effects model (MODEL B) on category, where problems were classified in terms of type of problem (e.g. time series, binary classification, etc).

We then ran a no pooling model (MODEL C), which is actually numerous separate models, one for each problem-type 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 diversity on performance, but the coefficient is small (less than .2) To interpret this result, an increase in l_1 diversity of one correponds to an increase of the z-score of the max score by less than 0.2.

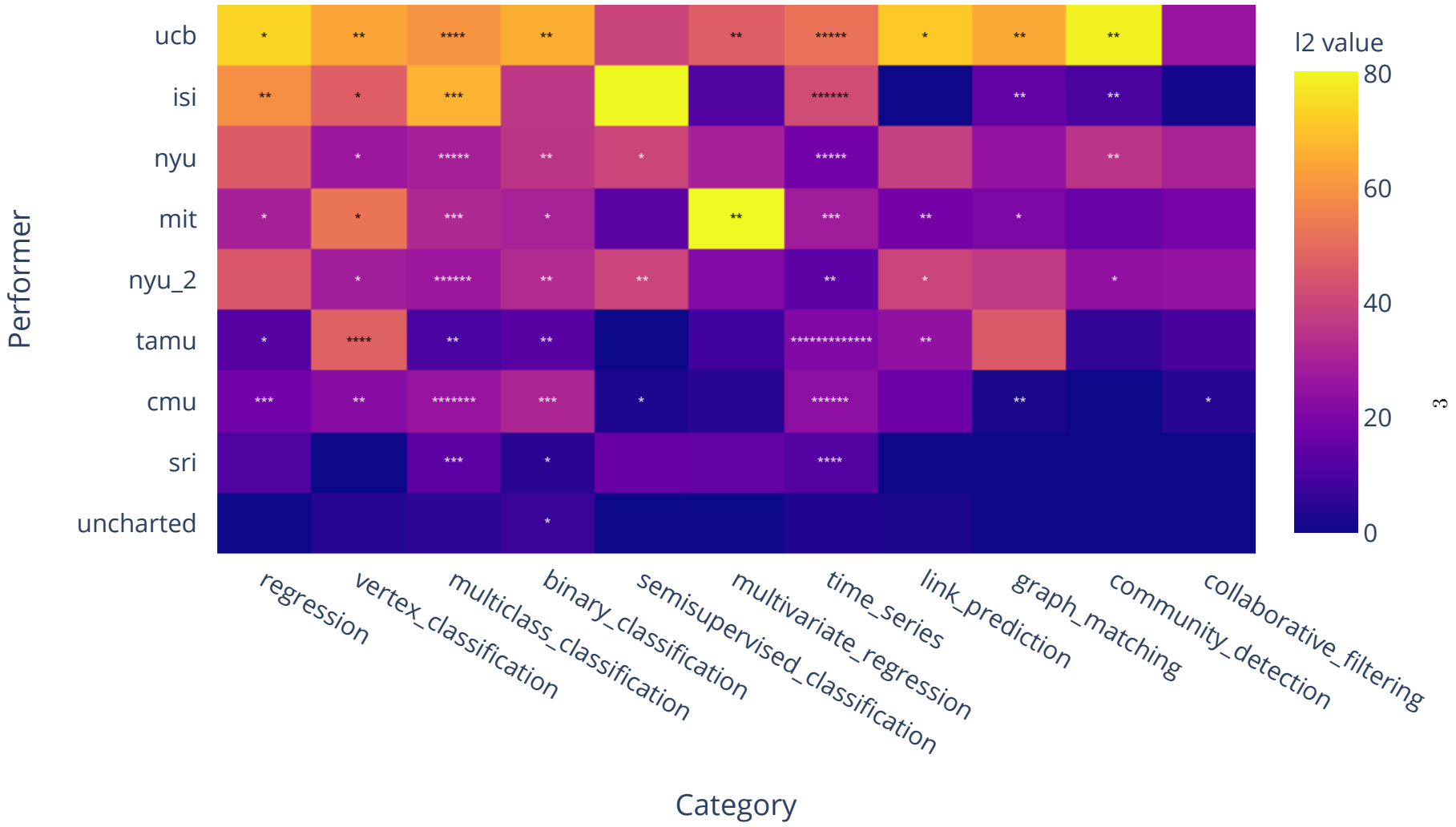


Figure 1: Heat map of l_2 diversity see section "Measures of Diversity" for a discussion of this and other measures we use to quantify diversity. The horizontal axis is the problem category and the vertical axis is performer for the Winter 2020 evaluation. The number of asterisks in each cell is the 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.

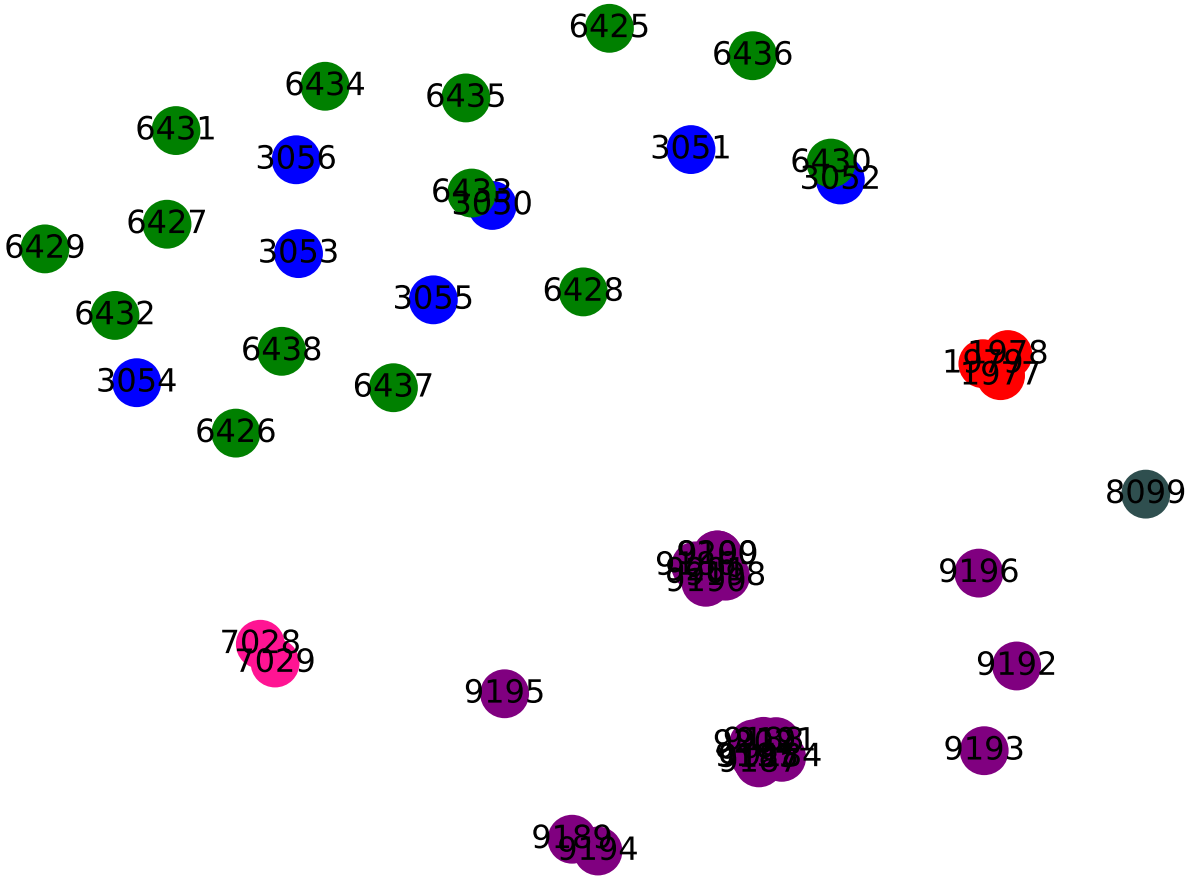
See Following Pages

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.

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).

SEMI_1217_click_prediction_small_MIN_METADATA



cmu	pipeline_1977	CX-SN----------IB----ZK-XD----------ZK-DD-LW-EX-GT-MM
cmu	pipeline_1978	CX-SN----------IB----ZK-XD----------ZK-DD-LW-EX-GT-MM
cmu	pipeline_1979	CX-SN----------IB----ZK-XD----------ZK-DD-LW-EX-GT-MM
nyu_2	pipeline_3050	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV----ZK-VK-GT-MM------
nyu_2	pipeline_3051	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-DD-ZK-ZK-LW-JP-EX----ZK-UA-MM---------
nyu_2	pipeline_3052	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-DD-ZK-ZK-LW-JP-EX----ZK-UO-MM---------
nyu_2	pipeline_3053	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV-EX-ZK-VK-GT-MM------
nyu_2	pipeline_3054	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV-NC-ZK-VK-GT-MM------
nyu_2	pipeline_3055	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-DD----ZK-VK-GT-MM------
nyu_2	pipeline_3056	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV-XN-ZK-VK-GT-MM------
nyu	pipeline_6425	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-DD-ZK-LW-ZK-JP-EX----ZK-UA-MM---------
nyu	pipeline_6426	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV-EX-ZK-OC-GT-MM------
nyu	pipeline_6427	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV-NC-ZK-OD-GT-MM------
nyu	pipeline_6428	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV----ZK-OC-GT-MM------
nyu	pipeline_6429	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----LW-ZK-JP-DD----ZK-VK-GT-MM------
nyu	pipeline_6430	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-DD-ZK-ZK-LW-JP-EX----ZK-UO-MM---------
nyu	pipeline_6431	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-DD-EX-ZK-YX-GT-MM------
nyu	pipeline_6432	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-DD-EX-ZK-OD-GT-MM------
nyu	pipeline_6433	CX-SN-HH-HH-HH-HH-HH-HH-XD-ZK-ZK----ZK-LW-JP-VV----ZK-VK-GT-MM------

SEMI_1217_click_prediction_small_MIN_METADATA

```
nyu        pipeline_6434 CX-SN-HH-HH-HH-HH-HH-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
OO: 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: lstm_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.sgm
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