Interpretable machine learning algorithms for understanding factors related to childhood autism

Toby Dylan Hocking toby.hocking@nau.edu toby.hocking@r-project.org

February 25, 2024

Motivation and data for predicting childhood autism

- We have data from the National Survey of Children's Health.
- ► Each year a number of people fill out the survey (rows), and we have data for their responses (columns).
- ▶ One column, k2q35a "Autism ASD" (Yes or No) represents if the child has Autism.
- Data pre-processing: operations prior to machine learning.
- Prediction accuracy in a given year: can we predict Autism variable (output/label/dependent), given the others? (inputs/features/independent)
- ► Model interpretation / feature selection: which inputs are most useful for prediction?
- ➤ Similarity/difference between years: Can we train on one survey year, and accurately predict on another?

Prediction accuracy in a given year

Model interpretation / feature selection

Similarity/difference between years

- Download NSCH data from public Census web site.
- ► For each year, keep all columns with less than 10% missing values, then remove all rows with at least one missing value.
- One-hot recoding of categorical variables (create 0/1 dummy/indicator variable for each value).
- ► Then keep only columns in common between both years: result is 46,010 rows and 366 columns. Details:

year	data.type	nrow	ncol	questions	%Autism	%rowsNA	%colsNA
2019	raw	29433	443	443	2.9615	100.0000	90.0677
2019	processed	18202	377	187	2.9997	0.0000	0.0000
2020	raw	42777	443	443	2.9758	100.0000	90.0677
2020	processed	27808	373	185	3.0818	0.0000	0.0000

Data source:

http://www2.census.gov/programs-surveys/nsch/datasets/2019/nsch_2019_topical_Stata.zip nsch_2019_topical.dta, nsch_2019_topical.do http://www2.census.gov/programs-surveys/nsch/datasets/2020/nsch_2020_topical_Stata.zip nsch_2020_topical.dta, nsch_2020_topical.do

One-hot encoding of categorical variables

Sometimes called dummy/indicator variables in statistics. For each value, we create a new column with 0/1 values. For example, from nsch_2020_topical.do

label var k4q24_r "Specialist Visit"
label define k4q24_r_lab 1 "Yes"
label define k4q24_r_lab 2 "No, but this child needed
to see a specialist", add
label define k4q24_r_lab 3 "No, this child did not
need to see a specialist", add

code above means there is a column named k4q24_r in nsch_2020_topical.dta, with values 1, 2, 3. In our analysis we use a one-hot encoding, which means deleting that column, and creating two 0/1 columns: Specialist Visit=Yes and Specialist Visit=No, but this child needed to see a specialist

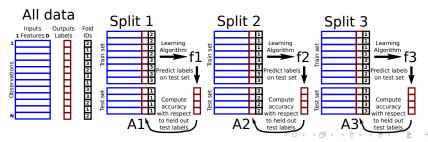
Prediction accuracy in a given year

Model interpretation / feature selection

Similarity/difference between years

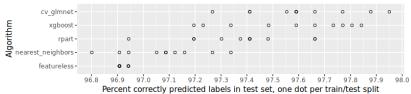
K-fold cross-validation: a standard algorithm used to estimate the prediction accuracy in machine learning

- K = 3 folds shown in figure below, meaning three different models trained, and three different prediction/test accuracy rates computed.
- It is important to use several train/test splits, so we can see if there are statistically significant differences between algorithms.
- Rows/observations are people, inputs/features are survey questions, and output/label is Autism response (Yes or No).



10-fold cross-validation for comparing learning algorithms





Learning algorithms we consider:

```
cv_glmnet L1-regularized linear model (feature selection).
```

xgboost Extreme gradient boosting (non-linear).

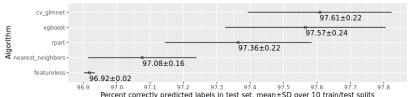
rpart Recursive partitioning, decision tree (non-linear, feature selection).

nearest_neighbors classic non-linear algorithm.

featureless un-informed baseline, ignores all inputs/features, and always predicts the most frequent label in train data (Autism=No in our case).

Summarize 10 folds with mean and standard deviation





Learning algorithms we consider:

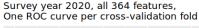
- cv_glmnet L1-regularized linear model (feature selection).
 - xgboost Extreme gradient boosting (non-linear).
 - rpart Recursive partitioning, decision tree (non-linear, feature selection).
- nearest_neighbors classic non-linear algorithm.
 - featureless un-informed baseline, ignores all inputs/features, and always predicts the most frequent label in train data (Autism=No in our case).

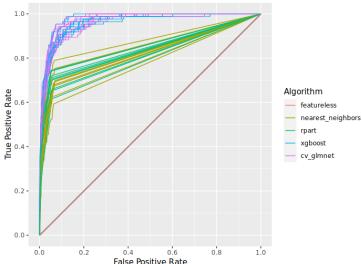
Confusion matrix and error rates

	Label 0	Label 1
Predict 0	True Negative (TN)	False Negative (FN)
Predict 1	False Positive (FP)	True Positive (TP)

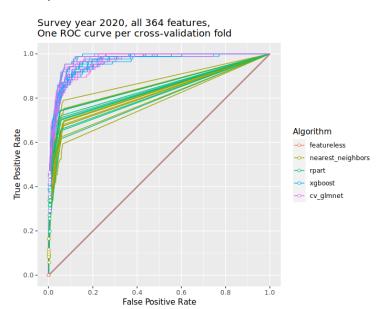
- ► Each has a corresponding rate which is a proportion between zero and one, for example FPR=False Positive Rate.
- Rates are related, TPR=1-FNR quantifies accuracy for positive labels, and TNR=1-FPR is for negative labels.
- ➤ TN/TP are good (want to maximize), whereas FP/FN are bad (want to minimize).
- ▶ Ideal rates are FPR=0 and TPR=1 but that is not possible to achieve in most real data.
- ▶ Receiver Operating Characteristic (ROC) curves trace TPR as a function of FPR, for every threshold of the learned prediction function f(x).

ROC curves show all tradeoffs between TPR and FPR

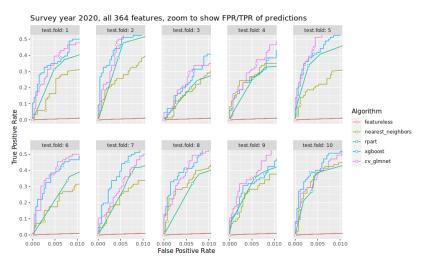




Default prediction threshold can be viewed as a dot

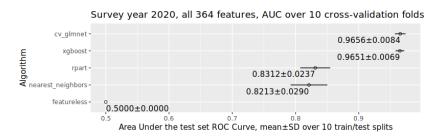


Default prediction threshold can be viewed as a dot



Relatively small FPR because there are so few positive labels (Autism=Yes only 3% of 27808 rows in 2020).

Area Under ROC Curve (AUC) quantifies accuracy over all thresholds



Prediction accuracy in a given year

Model interpretation / feature selection

Similarity/difference between years

Column categorization

Each input/feature column was assigned a category.

column_name,category
survey_year,
Autism,
State FIPS Code=Alabama,state

• • •

Number of Children in Household=1,home

. . .

Sex of Selected Child=Male, birth

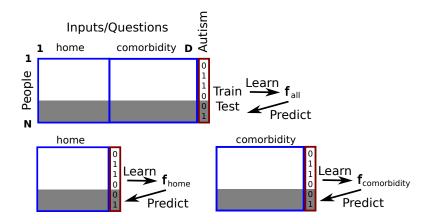
. . .

Deafness=Yes, comorbidity

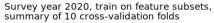
. . .

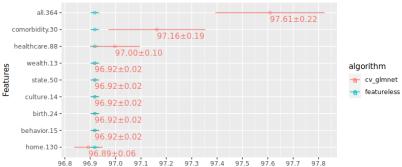
	behavior	birth	comorbidity
2	15	24	30
culture	healthcare	home	state
14	88	130	50
wealth			
4.0			

Cross-validation for category importance



Cross-validation for category importance



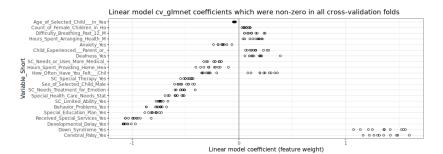


Percent correctly predicted labels in test set, mean±SD over 10 train/test splits

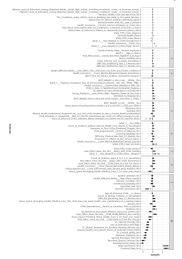
TODO equation

 Positive coefficients mean larger values of that feature are more likely to TODO

Linear model coefficient / feature importance



Linear model coefficient / feature importance



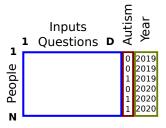
View full figure online, https:

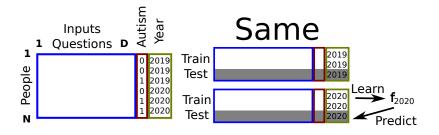
//github.com/tdhock/2024-01-ml-for-autism/blob/main/download-nsch-mlr3batchmark-registry-glmnet-coef.png

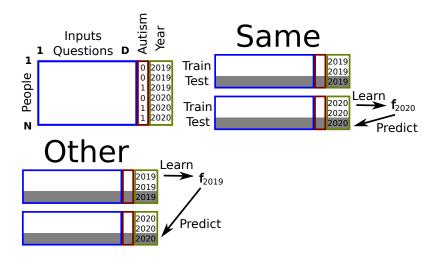
Prediction accuracy in a given year

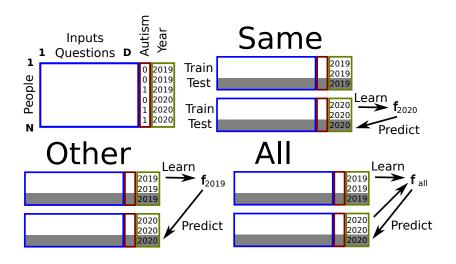
Model interpretation / feature selection

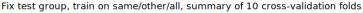
Similarity/difference between years

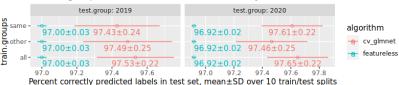












referre correctly predicted labels in test set, medit 150 over 10 train/test spirts

▶ 18,202 rows in 2019, whereas 27,808 in 2020.

Prediction accuracy in a given year

Model interpretation / feature selection

Similarity/difference between years

- ▶ Often we want to know if we have similar or different patterns in different groups (train on one year, predict on another).
- Cross-validation can be used to determine the extent to which we can train on one group, and accurately predict on another.
- ▶ Machine learning algorithms like L1 regularized linear models (LASSO/cv_glmnet) are additionally interpretable in terms of which features are used for prediction (can be compared between models trained on different groups).
- Free/open-source software available: mlr3resampling R package on CRAN and https://github.com/tdhock/mlr3resampling
- ► Let's collaborate! Contact: toby.hocking@nau.edu, toby.hocking@r-project.org