# Same vs. other cross-validation in supervsied machine learning

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Introduction to machine learning

Proposed same vs. other cross-validation

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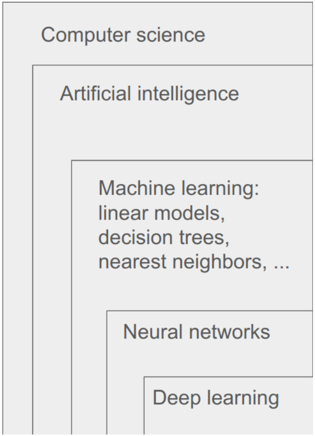
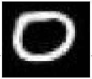
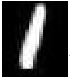
# What is machine learning?

- Computer science: domain of study about efficient algorithms / computations.
- Artificial intelligence: sub-domain concerned with algorithms for accurate predictions/suggestions.
- Machine learning: sub-domain concerned with algorithms for large data.
- Machine learning is widely used in search engines, automatic translation, image analysis, ...



# Machine learning intro: image classification example

ML is all about learning predictive functions $f(x) \approx y$, where

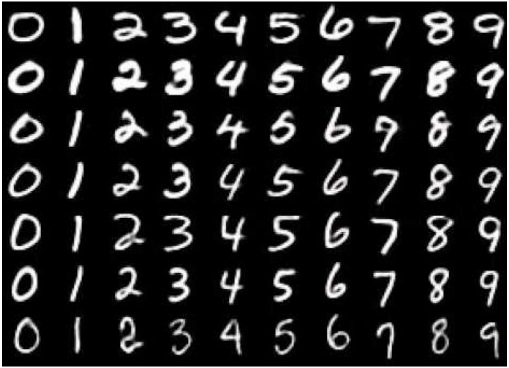
- Inputs/features $x$ can be easily computed using traditional algorithms, e.g. matrix of pixel intensities in an image.
- Outputs/labels $y$ are what we want to predict, easy to get by asking a human, but hard to compute using traditional algorithms, e.g. image class.
- Input $x =$ image of digit, output $y \in \{0, 1, \ldots, 9\}$,
  – this is a classification problem with 10 classes.
  $f($  $) = 0$, $f($  $) = 1$
- Traditional/unsupervised algorithm: I give you a pixel intensity matrix $x \in \mathbb{R}^{16 \times 16}$, you code a function $f$ that returns one of the 10 possible digits. Q: how to do that?

# Supervised machine learning algorithms

I give you a training data set with paired inputs/outputs, e.g.

$$y = 0\ 1\ 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9$$

$$X =$$



Your job is to code an algorithm that learns the function $f$ from the training data. (you don't code $f$)

Source: github.com/cazala/mnist

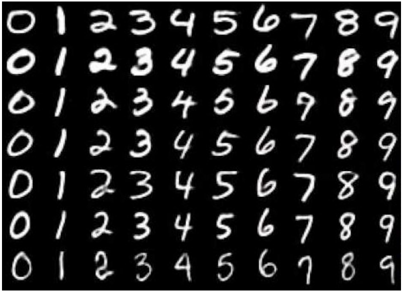
# Supervised machine learning algorithms

**Can** be used whenever a knowledgeable/skilled human can easily/quickly/consistently create a large database of labels for training.

**Should** be used if it is not easy to code the function $f$ for predicting the labels (using traditional/unsupervised techniques).

**Accurate** if the test data, on which you want to use $f$, is similar to the train data (input to learning algorithm).

# Advantages of supervised machine learning

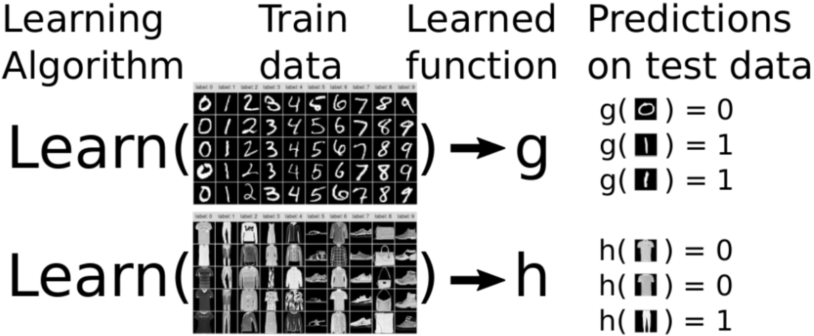


- Input $x \in \mathbb{R}^{16\times16}$, output $y \in \{0, 1, \ldots, 9\}$ types the same!
- Can use same learning algorithm regardless of pattern.
- Pattern encoded in the labels (not the algorithm).
- Useful if there are many un-labeled data, but few labeled data (or getting labels is long/costly).
- State-of-the-art accuracy (if there is enough training data).

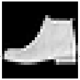
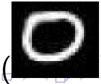
Sources: github.com/cazala/mnist, github.com/zalandoresearch/fashion-mnist

# Learning two different functions using two data sets

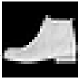
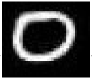
Figure from chapter by Hocking TD, *Introduction to machine learning and neural networks* for book *Land Carbon Cycle Modeling: Matrix Approach, Data Assimilation, and Ecological Forecasting* edited by Luo Y (Taylor and Francis, 2022).




**Learn** is a learning algorithm, which outputs $g$ and $h$.

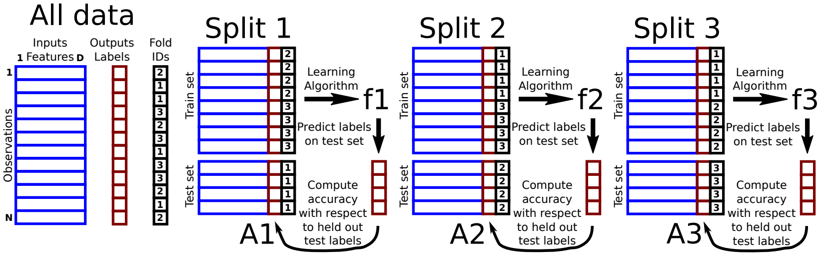
Q: what happens if you do $g($$)$, or $h($$)$?

# Learning two different functions using two data sets

- What if you do $g($$)$, or $h($$)$?
- This is a question about **generalization**: how accurate is the learned function on a new/test data set?
- "Very accurate" if test data are similar enough to train data (best case is i.i.d. = independent and identically distributed)
- Predicting childhood autism (Lindly *et al.*), train on one year of surveys, test on another.
- Predicting carbon emissions (Aslam *et al.*), train on one city, test on another.
- Predicting presence of trees/fires in satellite imagery (Shenkin *et al.*, *Thibault et al.*), train on one geographic area/image, test on another.
- Predicting fish spawning habitat in sonar imagery (Bodine *et al.*), train on one river, test on another.
- But how do we check if "very accurate" in these situations?

# $K$-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.



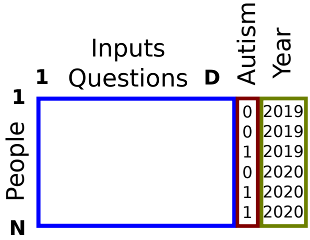

Hocking TD *Intro. to machine learning and neural networks* (2022).

# Example data set: predicting childhood autism

- Collaboration with Lindly *et al.*
- Downloaded National Survey of Children's Health (NSCH) data, years 2019 and 2020, from `http://www2.census.gov/programs-surveys/nsch`
- One row per person, one column per survey question.
- Pre-processing to obtain common columns over the two years, remove missing values, one-hot/dummy variable encoding.
- Result is $N = 46,010$ rows and $D = 366$ columns.
- 18,202 rows for 2019; 27,808 rows for 2020.
- One column is diagnosis with Autism (binary classification, yes or no), can we predict it using the others?
- Can we combine data from different years?
- Can we train on one year, and accurately predict on another?

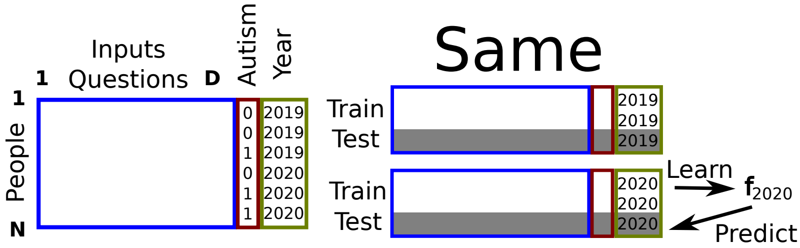
# Proposed Same Other Cross-Validation

- Example: childhood autism prediction data set.



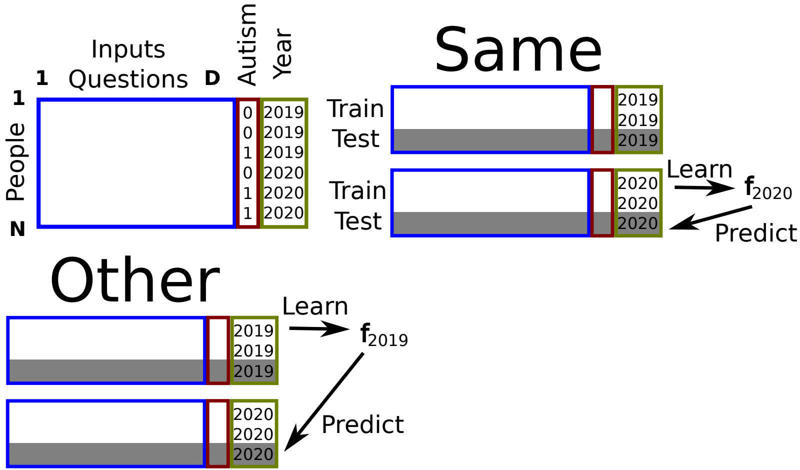
# Proposed Same Other Cross-Validation

- Train group same as test (=regular $K$-fold CV on 2020).



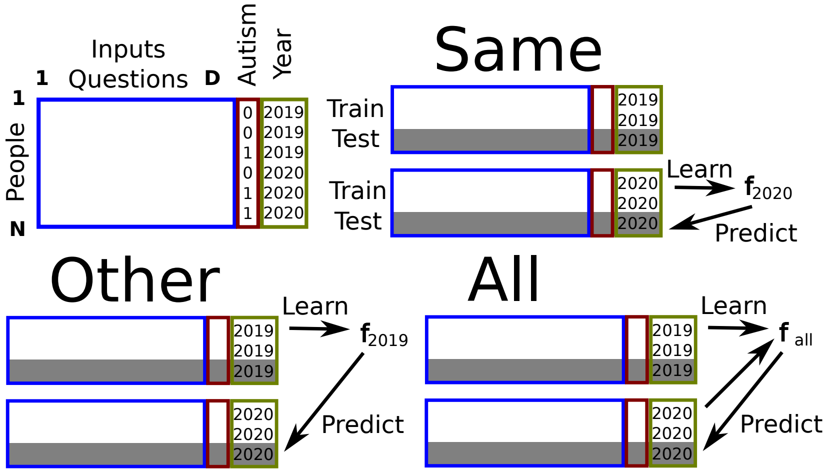
# Proposed Same Other Cross-Validation

- Train group (2019) different from test (2020).



# Proposed Same Other Cross-Validation

- Repeat for each of $K$ folds, and each test group (2019,2020).



# Proposed Same Other Cross-Validation

For a fixed test set from one group:
If train/test are similar/iid,

- **All** should be most accurate.
- **Same/Other** should be less accurate, because there is less data available (if other is larger than same, then other should be more accurate than same, etc).

If train/test are different (not iid),

- **Same** should be most accurate.
- **Other** should be substantially less accurate.
- **All** accuracy should be between same and other.

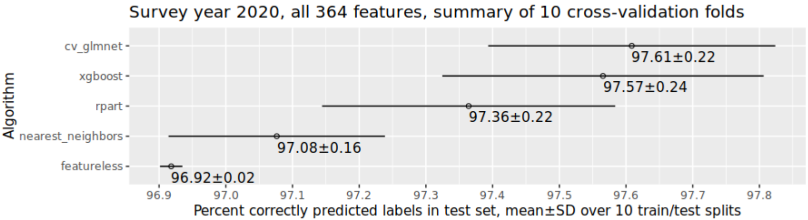
# Learning algorithms we consider

We used the following learning algorithms:

- **cv_glmnet** L1-regularized linear model (feature selection). Friedman, *et al.* (2010).
- **xgboost** Extreme gradient boosting (non-linear). Chen and Guestrin (2016).
- **rpart** Recursive partitioning, decision tree (non-linear, feature selection). Therneau and Atkinson (2023).
- **nearest_neighbors** classic non-linear algorithm, as implemented in kknn R package. Schliep and Hechenbichler (2016).
- **featureless** un-informed baseline, ignores all inputs/features, and always predicts the most frequent label in train data. For example, Autism=No. Nomenclature from mlr3 R package, Lang, *et al.*, (2019).

Each learning algorithm has different properties (non-linear, feature selection, etc). For details see Hastie, *et al.* (2009) textbook.

# $K$-fold CV on NSCH data (predict autism), year 2020




Learning algorithms we consider:

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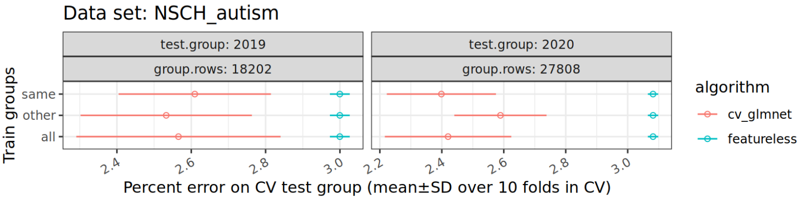
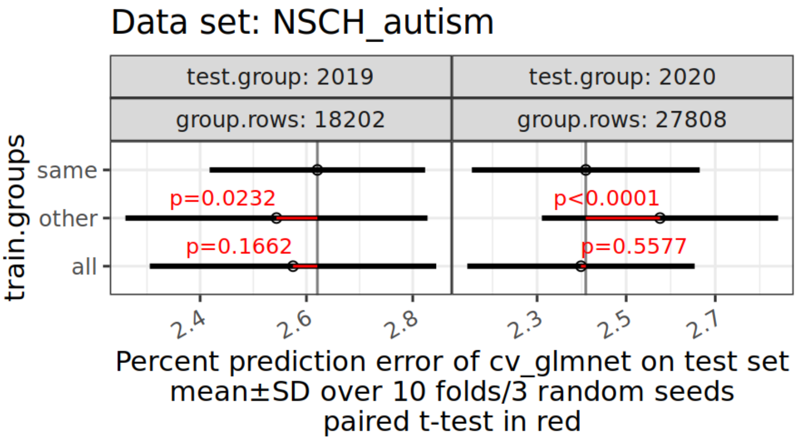
- **nearest_neighbors** classic non-linear algorithm.
- **featureless** un-informed baseline, ignores all inputs/features, and always predicts the most frequent label in train data (Autism=No in this case).

# Same Other CV for Autism data




- Each cv_glmnet model has significantly less error than featureless, indicating that some non-trivial pattern has been learned.

# Same Other CV for Autism data

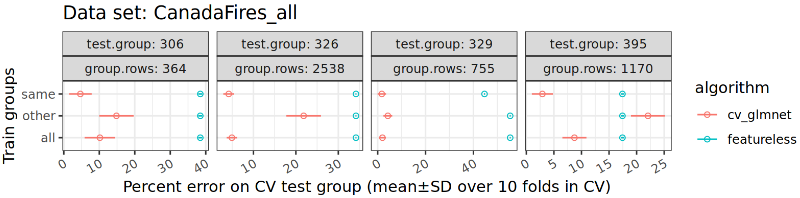



- All has slightly less error than same, which suggests the two years have similar patterns, and can be combined for learning a more accurate model.
- Other has either less error or more, suggesting that the error rate depends on the number of rows in the train set.

# Example data 2: Canada fires

- Collaboration with Thibault *et al.*
- Satellite image data, $N = 4827$ rows/pixels, $D = 46$ features/spectral bands.
- Government land management project: oal is to predict whether the pixel has been burned (binary classification, yes or no).
- Four satellite images in different regions of the forest, numbered 306, 326, 329, 395.
- Can we train on one image, and accurately predict on another?

# Same Other CV for Canada fires data

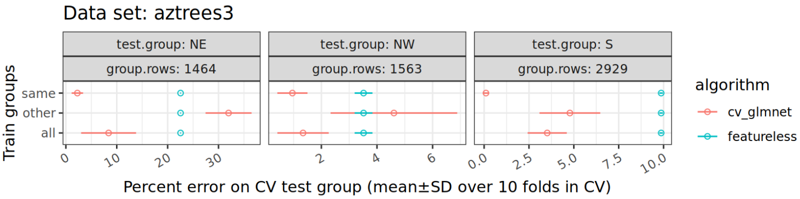



- Each cv_glmnet model has significantly less error than featureless, except train.groups=other for test.group=395 (must have a very different pattern than the other images).
- Training on all images is never as accurate as same, which suggests that images are substantially different, and we need labels from the same image to get optimal predictions.

# Example data 3: AZ trees

- Collaboration with Shenkin *et al.*
- Satellite image data, $N = 5956$ rows/pixels, $D = 21$ features/spectral bands.
- Tree stress project: goal is to predict whether the pixel has a tree (binary classification, yes or no).
- Three regions around Flagstaff: NE, NW, S.
- Can we train in one region, and accurately predict on another?

# Same Other CV for AZ trees data

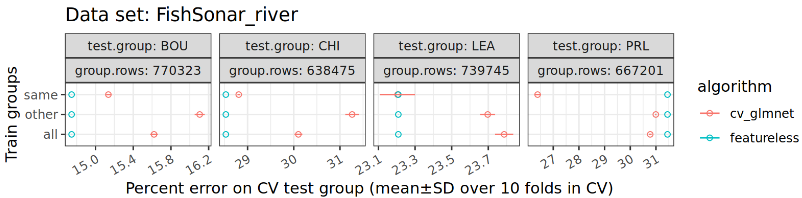



- Each cv_glmnet model has significantly less error than featureless, except train.groups=other for two test groups (must have a very different pattern than the other images).
- Training on all images is never as accurate as same, which suggests that images are substantially different, and we need labels from the same image to get optimal predictions.

# Example data 4: fish sonar

- Collaboration with Bodine *et al.*
- Sonar image data, $N = 2,815,744$ rows/pixels, $D = 81$ features (mean pixel intesity in windows around target pixel).
- Conservation project funded by Department of Fish/Wildlife: goal is to predict whether the pixel has a hard bottom suitable for fish spawning (binary classification, yes or no).
- Four rivers in southeast USA: CHI, PRL, LEA, BOU.
- Can we train in one river, and accurately predict on another?

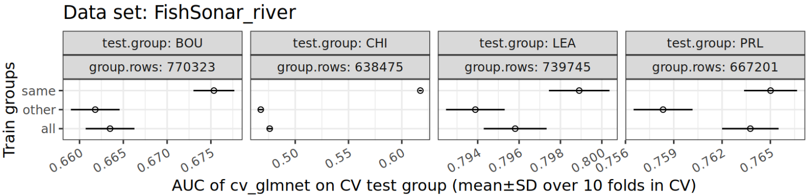
# Same Other CV for fish sonar data




- When training on same group, cv_glmnet sometimes has larger test error than featureless, because of class imbalance (hard bottom suitable for fish spawning is rare).

```
       river
label      BOU    CHI    LEA    PRL
  hard  113592 182150 171684 209832
  other 656731 456325 568061 457369
```

# Same Other CV for fish sonar data




- Area Under the ROC Curve (AUC) is a good measure of accuracy for imbalanced binary classification problems (constant/featureless=0.5, best=1).
- Mostly test AUC is greater than 0.5, which means a non-trivial prediction function has been learned.
- For test.group=CHI with train.groups=all/other, test AUC$<$ 0.5, indicating a very different pattern in this river (opposite of the pattern in other rivers).
- Test AUC for all is never as large as same, indicating that you need data from the same river for optimal prediction accuracy.

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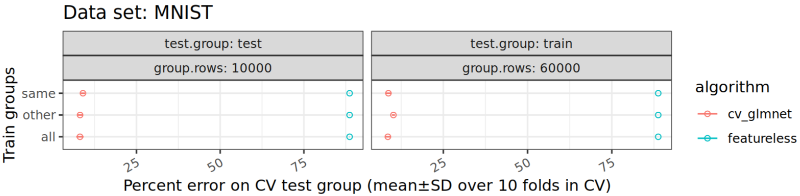
# Machine learning benchmark data sets

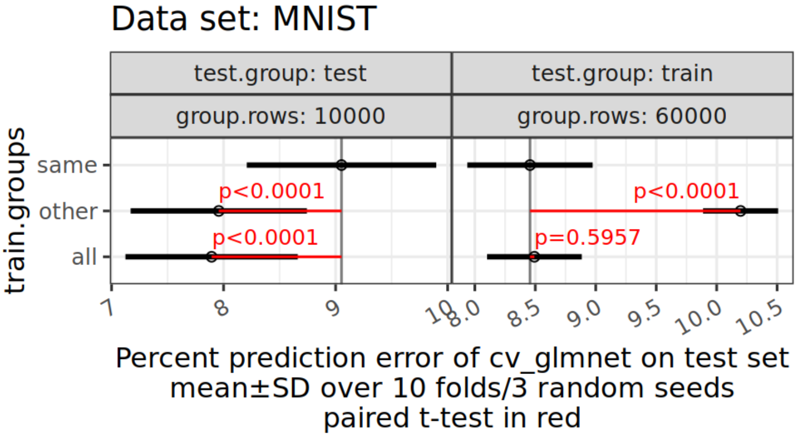
- Machine learning researchers evaluate new algorithms using benchmark data sets, which sometimes have pre-defined train/test splits.
- For example MNIST is a data set of images of handwritten digits (want to predict which digit, 0 to 9), with 60,000 train and 10,000 test images.
- spam is a data set of emails (want to predict spam or not, binary), with 3065 train and 1536 test emails.
- Are the patterns in the pre-defined train/test sets similar/iid?
- Or are they different?

# Same Other CV for MNIST data



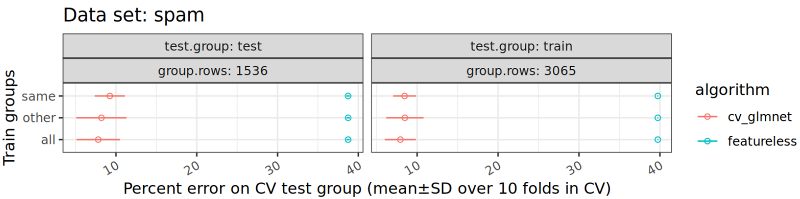

- TODO

# Same Other CV for MNIST data



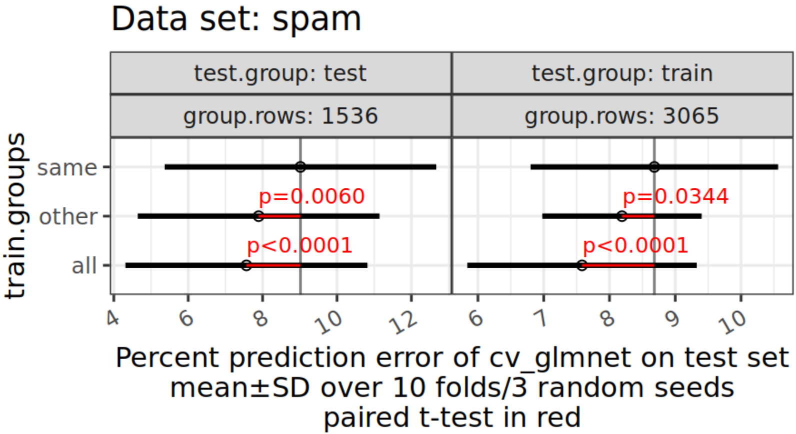

- TODO

# Same Other CV for spam data



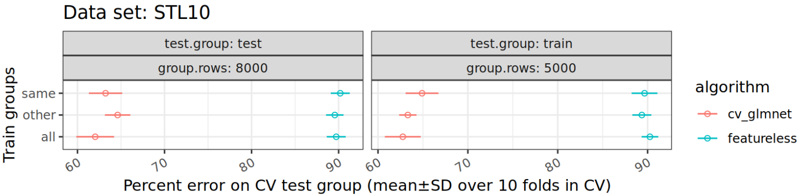

- TODO

# Same Other CV for spam data



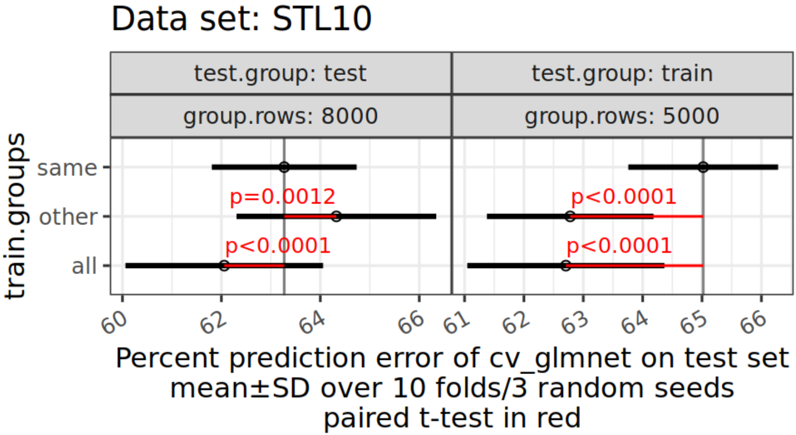

- TODO

# Same Other CV for STL10 data



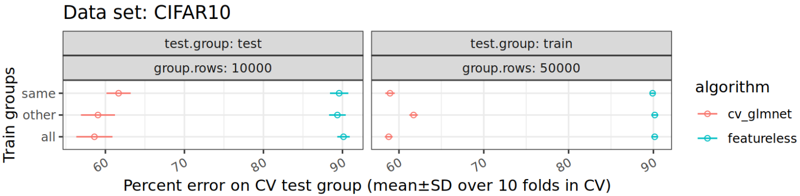

- TODO

# Same Other CV for STL10 data



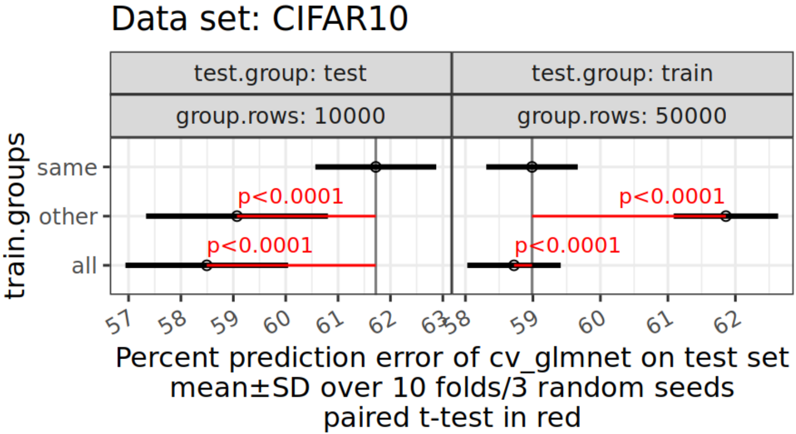

- TODO

# Same Other CV for CIFAR10 data




- TODO

# Same Other CV for CIFAR10 data

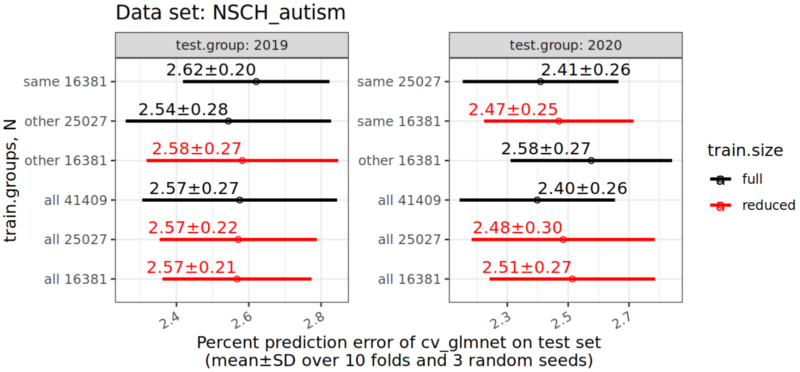



- TODO

# Discussion and Conclusions

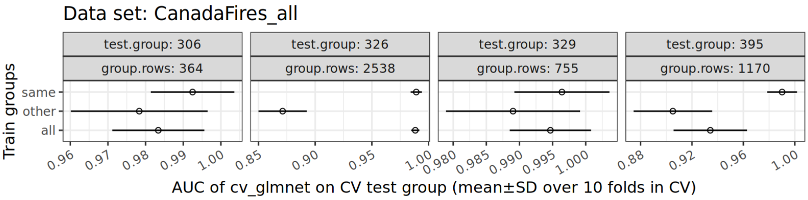
- Proposed Same Other Cross-Validation can be used to see if data sets are similar enough to so that combining data is beneficial for training (train on one group, test/predict on another).
- In Autism data, there was a slight benefit to combining years.
- In image classification data (fires/trees/fish), we observed significant differences between images/regions/rivers.
- Free/open-source R package available: `https://github.com/tdhock/mlr3resampling`
- These slides are reproducible, using the code in `https://github.com/tdhock/cv-same-other-paper`
- Contact: toby.hocking@nau.edu, toby.hocking@r-project.org

# Same Other CV for Autism data




- Reduced sizes (red) are used to judge the effect of sample size.
- Sample size effect present for test group 2020, but not 2019.

# Same Other CV for Canada fires data




- Area Under the ROC Curve (AUC) is a good measure of accuracy for imbalanced binary classification problems (constant/featureless=0.5, best=1).
- Test AUC for all is never as large as same, indicating that you need data from the same river for optimal prediction accuracy.

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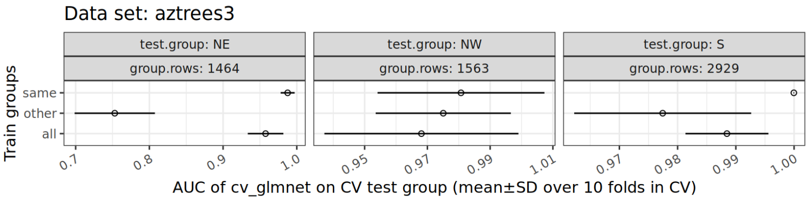


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