

Same vs. other cross-validation in supervised machine learning

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Introduction to machine learning

Proposed same vs. other cross-validation

Results on real data sets

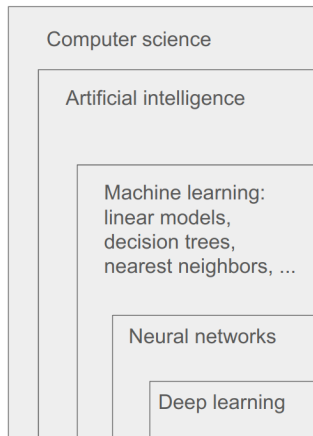
Results on machine learning benchmark data sets

Discussion and Conclusions

Supplementary slides

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

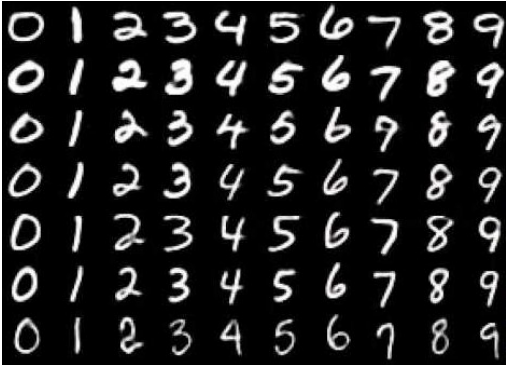
- ▶ Inputs/features x can be easily computed using traditional algorithms, e.g. matrix of pixel intensities in an image.
- ▶ Outputs/labels y are what we want to predict, easy to get by asking a human, but hard to compute using traditional algorithms, e.g. image class.
- ▶ Input x = image of digit, output $y \in \{0, 1, \dots, 9\}$,
 - this is a classification problem with 10 classes.

$f(\text{image of 0}) = 0, f(\text{image of 1}) = 1$

- ▶ 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.

$$y = \begin{matrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{matrix}$$

$$X =$$

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

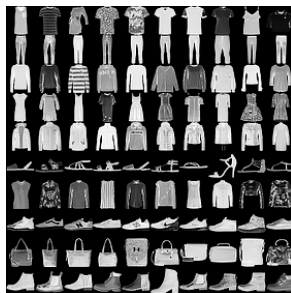
Supervised machine learning algorithms

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 $x \in \mathbb{R}^{16 \times 16}$, output $y \in \{0, 1, \dots, 9\}$ 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).

Learning Algorithm	Train data	Learned function	Predictions on test data
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Learn() → g	$g(\text{0}) = 0$ $g(\text{1}) = 1$ $g(\text{1}) = 1$
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Learn() → h	$h(\text{shirt}) = 0$ $h(\text{shirt}) = 0$ $h(\text{pants}) = 1$
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Learn is a learning algorithm, which outputs g and h .



Q: what happens if you do $g(\text{shoe})$, or $h(\text{ring})$?

Learning two different functions using two data sets



- ▶ What if you do $g(\text{shoe})$, or $h(\text{ring})$?
- ▶ 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?

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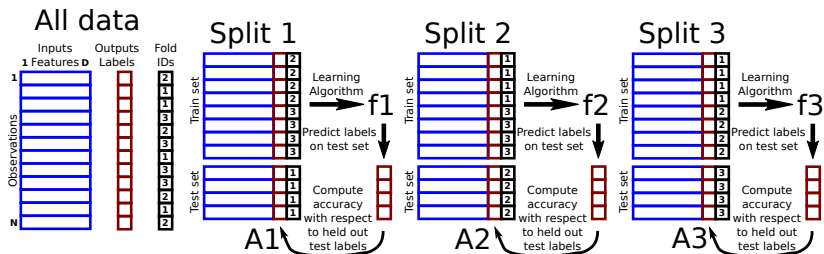
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K -fold cross-validation: a standard algorithm used to estimate the prediction accuracy in machine learning

- ▶ $K = 3$ 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.



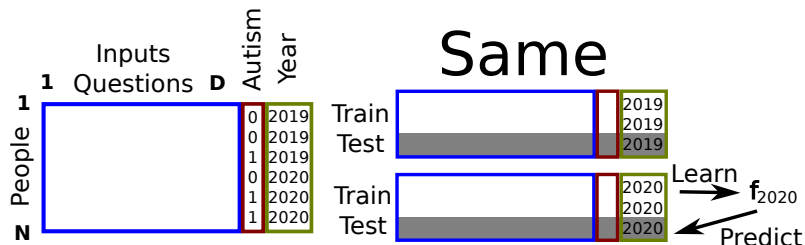
Hocking TD *Intro. to machine learning and neural networks* (2022).

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?

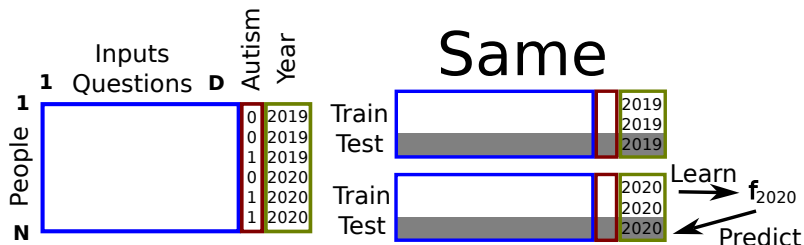
Proposed Same Other Cross-Validation

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

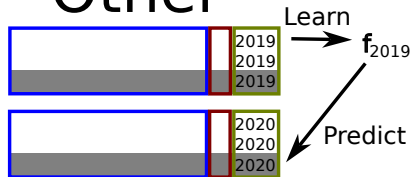


Proposed Same Other Cross-Validation

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

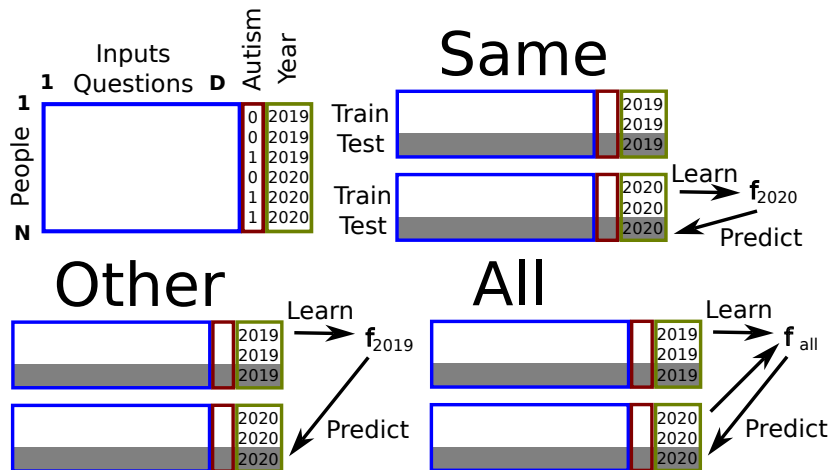


Other



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.

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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).

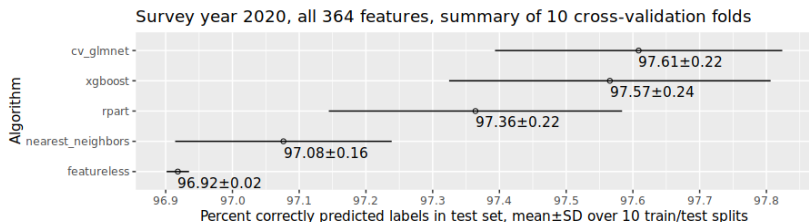
`rpart` Recursive partitioning, decision tree (non-linear,
feature selection). Therneau and Atkinson (2023).

`nearest_neighbors` classic non-linear algorithm, as implemented in
knnn 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:

cv_glmnet L1-regularized linear model (feature selection).

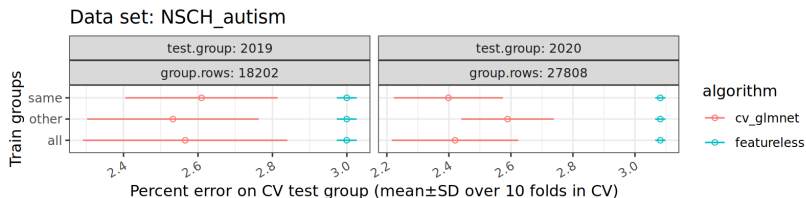
xgboost Extreme gradient boosting (non-linear).

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 this case).

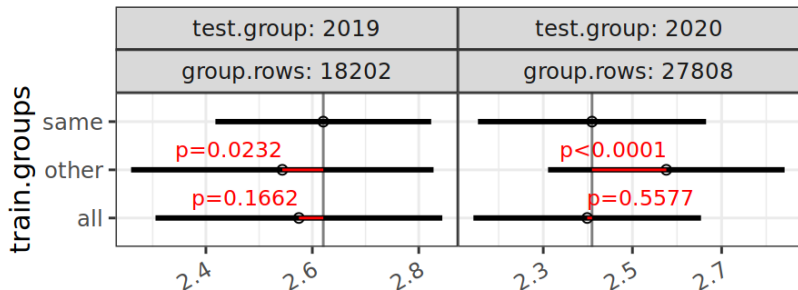
Same Other CV for Autism data



- 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

Data set: NSCH_autism

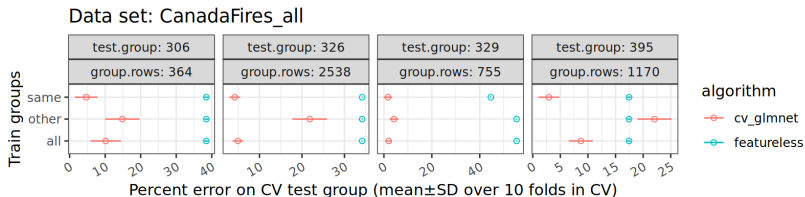


- ▶ All has slightly less error than same, which suggests the two years have similar patterns, and can be combined for learning a more accurate model.
- ▶ Other has either less error or more, suggesting that the error rate depends on the number of rows in the train set.

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: goal 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

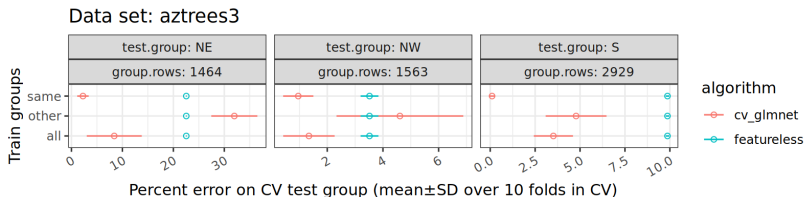


- ▶ Each cv_glmnet model has significantly less error than featureless, except train.groups=other for test.group=395 (must have a very different pattern than the other images).
- ▶ Training on all images is never as accurate as same, which suggests that images are substantially different, and we need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

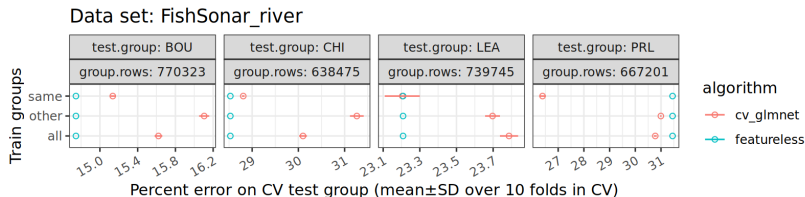


- ▶ Each cv_glmnet model has significantly less error than featureless, except train.groups=other for two test groups (must have a very different pattern than the other images).
- ▶ Training on all images is never as accurate as same, which suggests that images are substantially different, and we need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

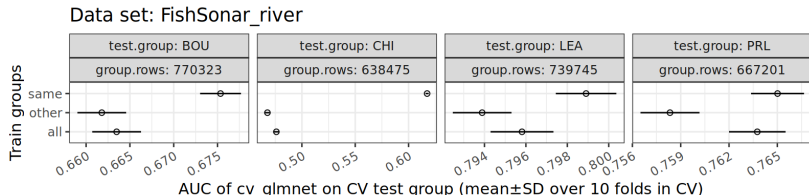
Same Other CV for fish sonar data



- ▶ 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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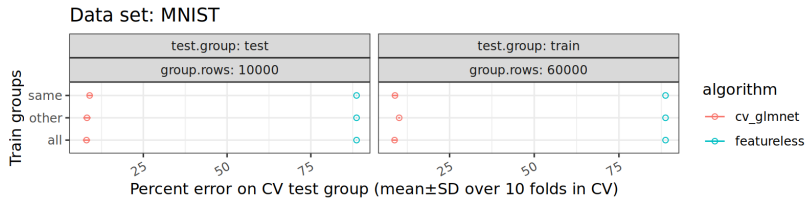
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Supplementary slides

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?

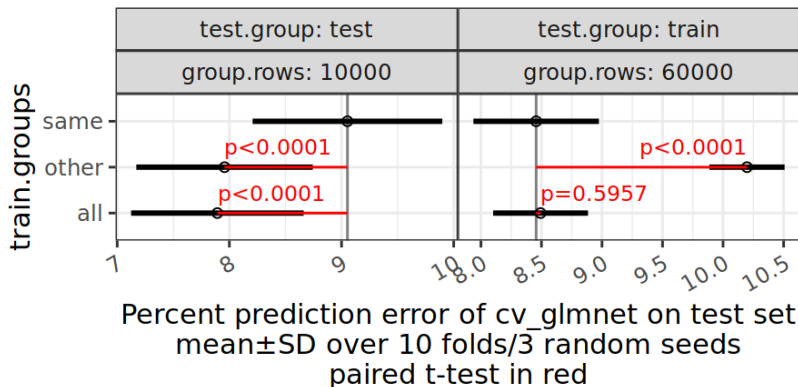
Same Other CV for MNIST data



► TODO

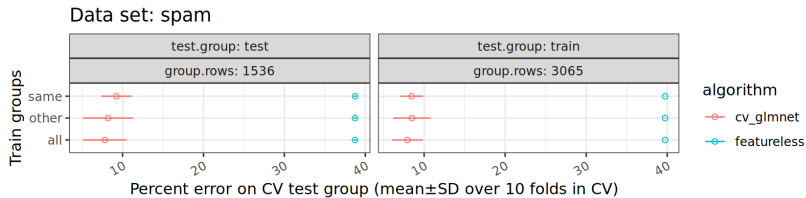
Same Other CV for MNIST data

Data set: MNIST



► TODO

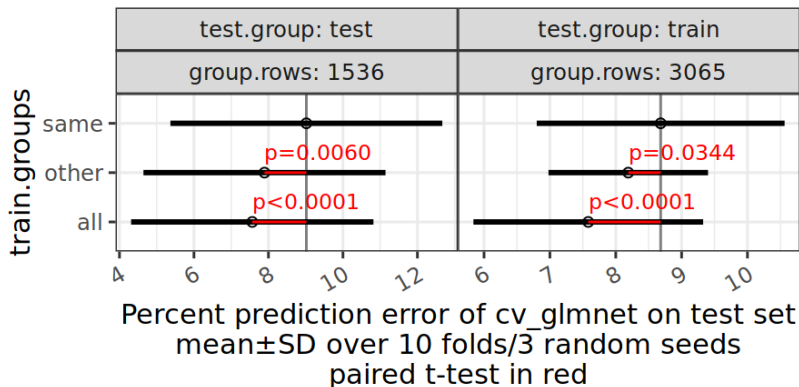
Same Other CV for spam data



► TODO

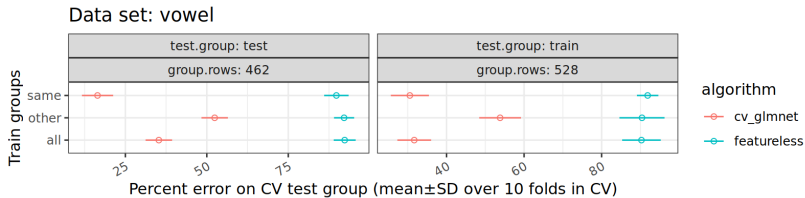
Same Other CV for spam data

Data set: spam



► TODO

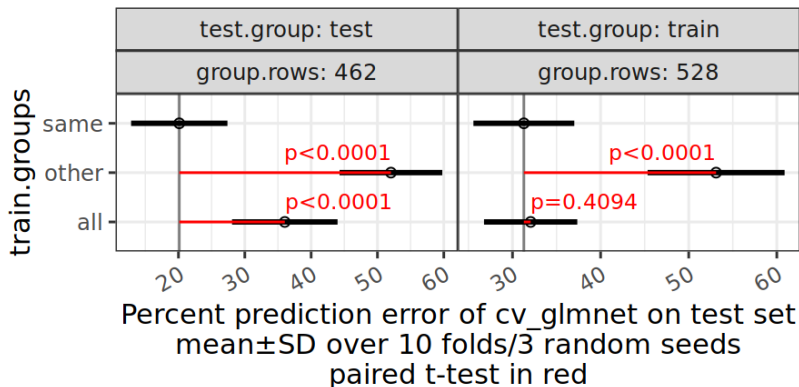
Same Other CV for vowel data



► TODO

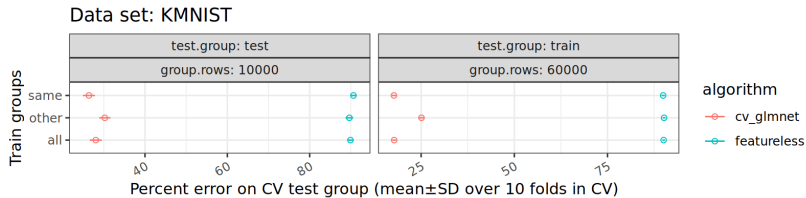
Same Other CV for vowel data

Data set: vowel



► TODO

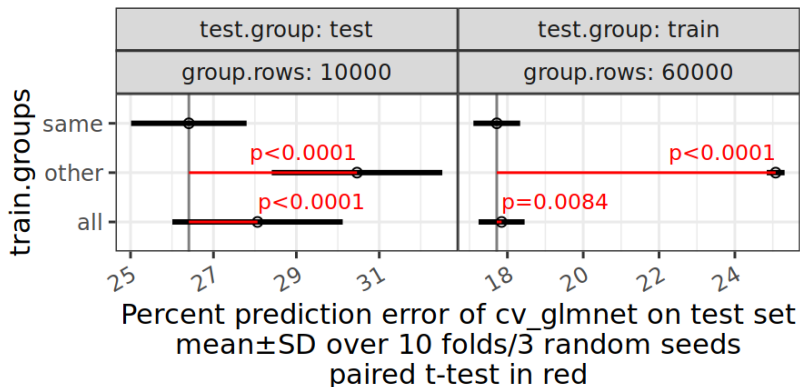
Same Other CV for KMNIST data



► TODO

Same Other CV for KMNIST data

Data set: KMNIST

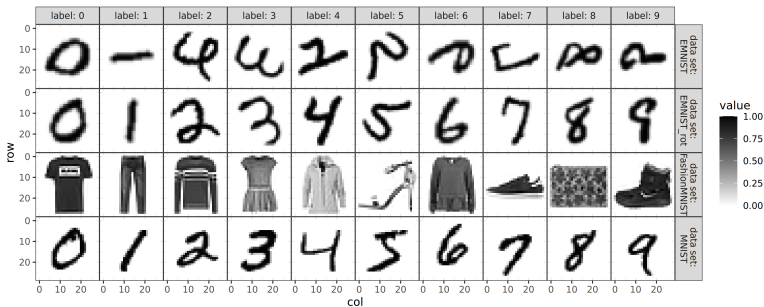


► TODO

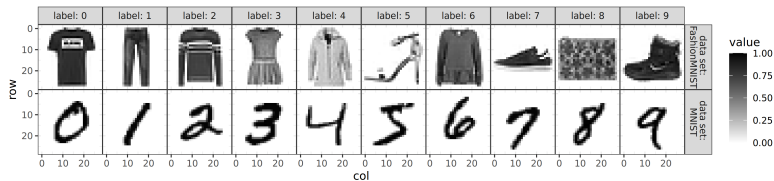
Train on MNIST and accurately predict on EMNIST?

Recall: what happens if you do $g(\text{boot image})$, or $h(\text{0 image})$?

- ▶ Boot image comes from FashionMNIST data, which were used to learn h .
- ▶ 0 image comes from MNIST data, which were used to learn g .



Same Other CV for MNIST+FashionMNIST data

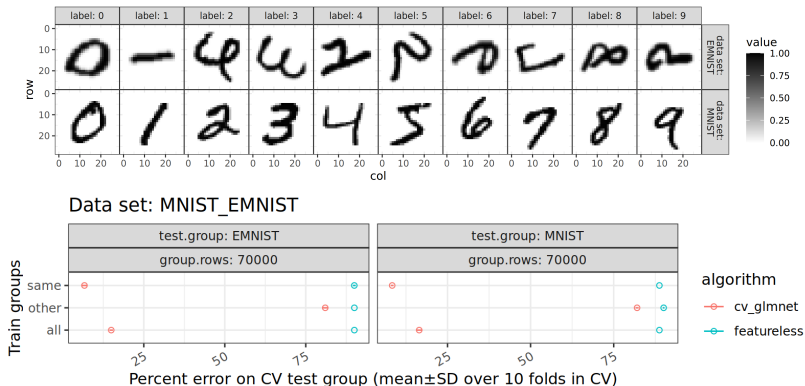


Data set: MNIST_FashionMNIST



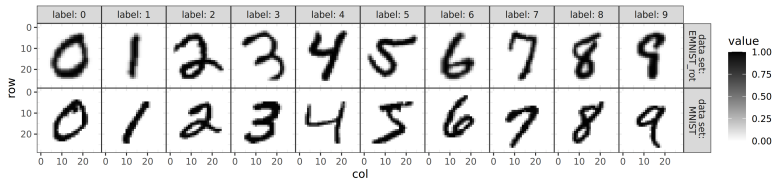
► TODO

Same Other CV for MNIST+EMNIST data



► TODO

Same Other CV for MNIST+EMNIST_rot data



► TODO

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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

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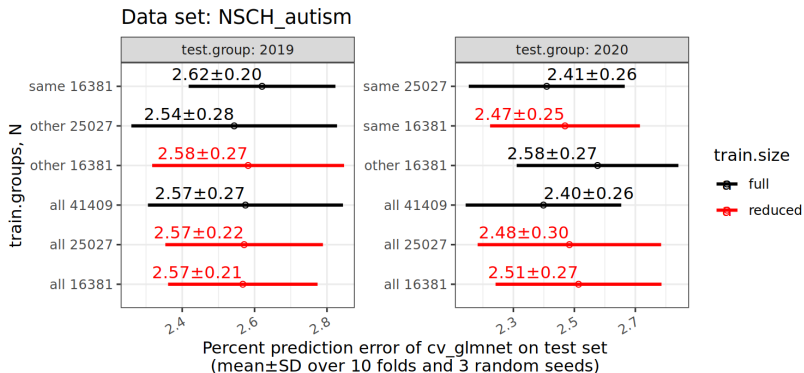
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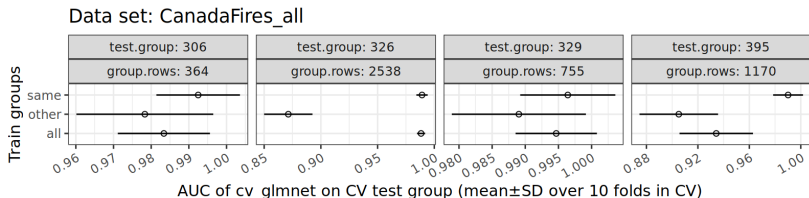
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Same Other CV for Autism data



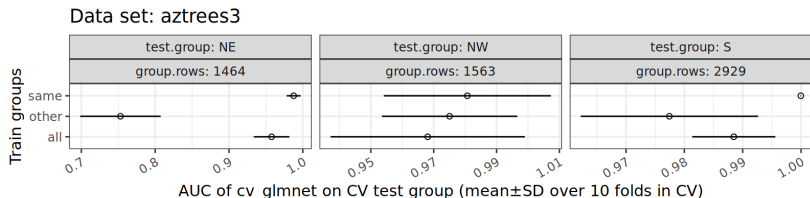
- ▶ Reduced sizes (red) are used to judge the effect of sample size.
- ▶ Sample size effect present for test group 2020, but not 2019.

Same Other CV for Canada fires data



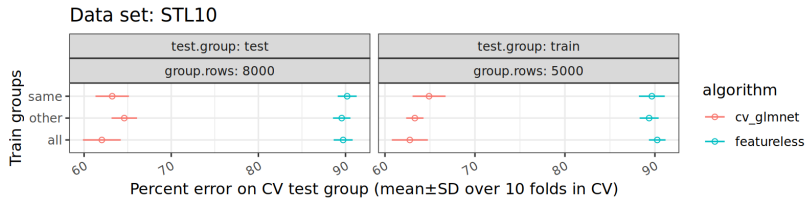
- ▶ Area Under the ROC Curve (AUC) is a good measure of accuracy for imbalanced binary classification problems (constant/featureless=0.5, best=1).
- ▶ Test AUC for all is never as large as same, indicating that you need data from the same river for optimal prediction accuracy.

Same Other CV for AZ trees data



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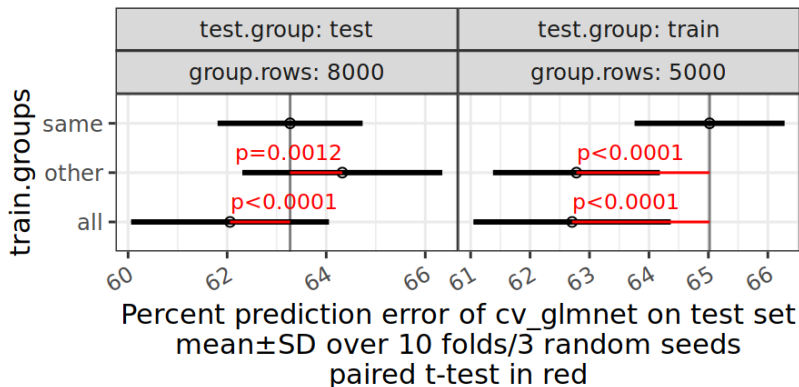
Same Other CV for STL10 data



► TODO

Same Other CV for STL10 data

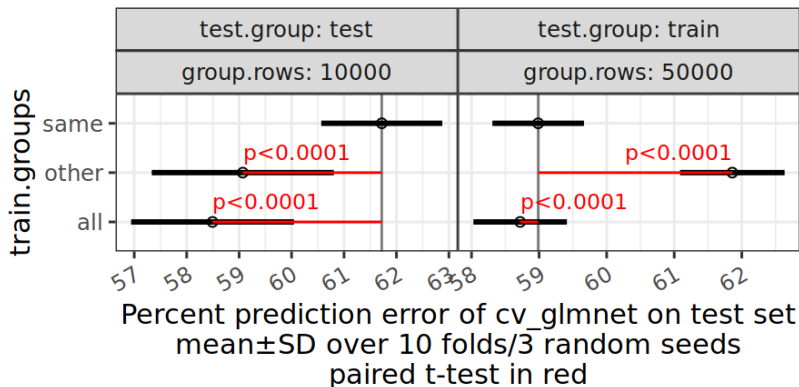
Data set: STL10



► TODO

Same Other CV for CIFAR10 data

Data set: CIFAR10



► TODO