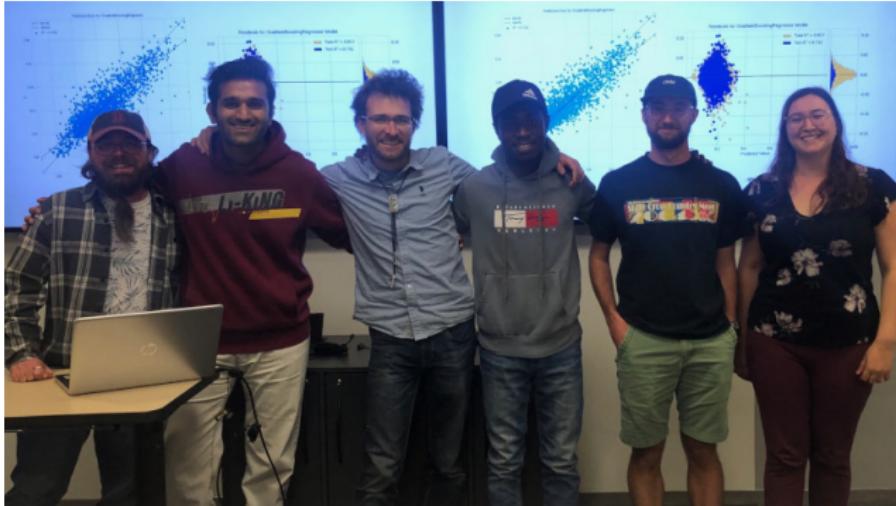


# Two new algorithms for scientific applications of machine learning

Toby Dylan Hocking — [toby.dylan.hocking@usherbrooke.ca](mailto:toby.dylan.hocking@usherbrooke.ca)

Learning Algorithms, Statistical Software, Optimization  
(LASSO Lab) — <https://lassolab.org>

Département d'Informatique, Université de Sherbrooke



## Introduction: two common questions in collaborations involving scientific applications of machine learning

Train on one subset and accurately predict on another?

SOAK: Same/Other/All K-fold cross-validation for estimating similarity of patterns in data subsets (arXiv:2410.08643)

How to deal with class imbalance?

AUM: Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization (JMLR'23)

# 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                                    |
|--------------------|---|------------------|---|
| Learn(             |  | $\rightarrow g$  | $g(\text{0}) = 0$<br>$g(\text{1}) = 1$<br>$g(\text{1}) = 1$ |
| Learn(             |  | $\rightarrow h$  | $h(\text{1}) = 0$<br>$h(\text{1}) = 0$<br>$h(\text{1}) = 1$ |

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

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



## Train on one subset and accurately predict on another?

- ▶ This is a question about **generalization**: how accurate is the learned function on a new/test data subset which is **qualitatively different** in some respect?
- ▶ “Very accurate” if test data are similar enough to train data (best case is i.i.d. = independent and identically distributed)



- ▶ What if you do  $g(\text{[image]})$ , or  $h(\text{[image]})$ ? (**different pattern**)
- ▶ Predicting childhood autism (Lindly *et al.*), train on one year of surveys, test on another. (**different time periods**)
- ▶ Predicting carbon emissions (Aslam *et al.*), train on one city, test on another. (**different geographic regions**)
- ▶ Predicting presence of trees/burn in satellite imagery (Shenkin *et al.*, Thibault *et al.*), train on one geographic area/image, test on another. (**different geographic regions**)
- ▶ Predicting fish spawning habitat in sonar imagery (Bodine *et al.*), train on one river, test on another. (**geographic regions**)
- ▶ But how do we check if “very accurate” in each situation?

## How to deal with class imbalance?

- ▶ In binary classification, standard learning algorithms can yield sub-optimal prediction accuracy if train data have imbalanced labels.
- ▶ Predicting childhood autism (Lindly *et al.*), 3% autism, 97% not.
- ▶ Predicting presence of trees/burn in satellite imagery (Shenkin *et al.*, Thibault *et al.*), small percent of trees in deserts of Arizona, small percent of burned area out of total forested area in Quebec.
- ▶ Predicting fish spawning habitat in sonar imagery (Bodine *et al.*), small percent of suitable spawning habitat, out of total river bed.
- ▶ How do we adapt our learning algorithm, to handle the class imbalance?

Introduction: two common questions in collaborations involving scientific applications of machine learning

Train on one subset and accurately predict on another?

SOAK: Same/Other/All K-fold cross-validation for estimating similarity of patterns in data subsets (arXiv:2410.08643)

How to deal with class imbalance?

AUM: Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization (JMLR'23)

## Example data with subsets: 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 ( $N = 46,010$  rows), one column per survey question ( $D = 366$  columns).
- ▶ Output/label column is diagnosis with Autism (binary classification, yes or no),  
can we predict it using the 365 inputs/features?
- ▶ 18,202 rows for 2019; 27,808 rows for 2020.

Proposed SOAK algorithm is a generalization of standard K-fold cross-validation, that can be used to answer two related questions:

- ▶ Can we train on one year, and accurately predict on another?
- ▶ Can we get a more accurate model by combining data from different years?

# K-fold cross-validation: a standard algorithm used to estimate 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).

## Proposed SOAK algorithm (Autism data example)

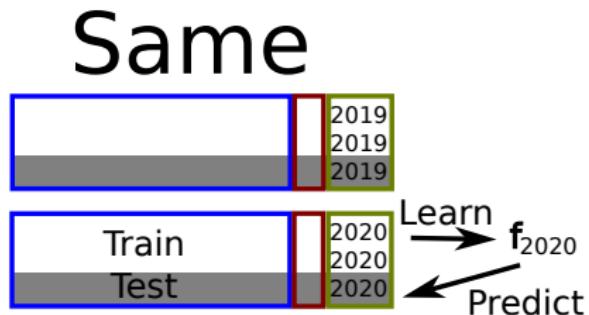
- ▶ Example: childhood autism prediction data set.
- ▶ Subsets of interest are years, which can be represented by adding a new column to the data table.

| Inputs | Autism    | Year   |
|--------|-----------|--------|
| 1      | Questions | 0 2019 |
| 1      |           | 0 2019 |
|        |           | 1 2019 |
|        |           | 0 2020 |
|        |           | 1 2020 |
|        |           | 1 2020 |

# Proposed SOAK algorithm (Autism data example)

- ▶ Train subset same as test (=regular  $K$ -fold CV on 2020).
- ▶ Do we get a more or less accurate model than this baseline  
Same model? (if we train on Other/All years)

| Inputs<br>Questions | D | Autism | Year |
|---------------------|---|--------|------|
| 1                   |   |        |      |
|                     | 0 | 2019   |      |
|                     | 0 | 2019   |      |
|                     | 1 | 2019   |      |
|                     | 0 | 2020   |      |
|                     | 1 | 2020   |      |
|                     | 1 | 2020   |      |



# Proposed SOAK algorithm (Autism data example)

- ▶ Test subset fixed (2020), train on other subset/year (2019).
- ▶ Can we train on one year, and accurately predict on another?  
Compare Same/Other test error.

| People | Inputs<br>Questions | D | Autism | Year |
|--------|---------------------|---|--------|------|
|        |                     |   | 1      | N    |
| 1      |                     |   | 0      | 2019 |
|        |                     |   | 0      | 2019 |
|        |                     |   | 1      | 2019 |
|        |                     |   | 0      | 2020 |
|        |                     |   | 1      | 2020 |
|        |                     |   | 1      | 2020 |

## Other

| Train | Test | 2019 | 2020 |
|-------|------|------|------|
|       |      | 2019 | 2019 |
|       |      | 2019 | 2020 |



## Same

| Train | Test | 2019 | 2020 |
|-------|------|------|------|
|       |      | 2019 | 2020 |
|       |      | 2019 | 2020 |

Learn  $\rightarrow f_{2020}$

Predict

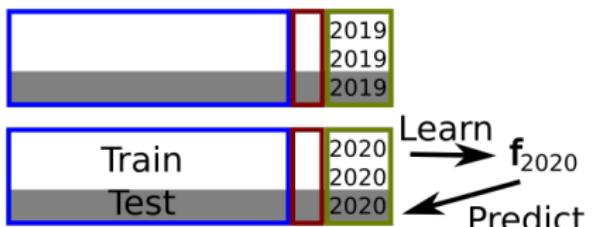
- Compare Same and Other error when predicting on test subset (2020)
- If subsets are similar, (2019 data are useful for learning how to predict in 2020) then the larger subset (Same or Other) should have smaller test error

# Proposed SOAK algorithm (Autism data example)

- ▶ Train set includes data from both subsets/years (2019, 2020).
- ▶ Can we get a more accurate model by combining data from different years? Compare Same/All test error.

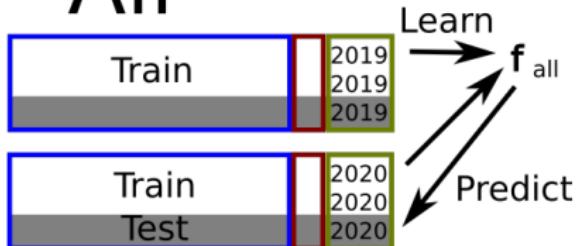
| People | Inputs<br>Questions | D | Autism | Year |
|--------|---------------------|---|--------|------|
|        |                     |   | 1      | N    |
| 1      |                     |   | 0      | 2019 |
|        |                     |   | 0      | 2019 |
|        |                     |   | 1      | 2019 |
|        |                     |   | 0      | 2020 |
|        |                     |   | 1      | 2020 |
|        |                     |   | 1      | 2020 |

## Same



- Compare Same and All error when predicting on test subset (2020)
- If subsets are similar, (2019+2020 data are useful for learning how to predict in 2020) then All test error should be less than Same (more relevant data available)

## All



# Proposed SOAK algorithm (generic data)

- ▶ Key new idea is **subset** column in data table.
- ▶ Example:  $K = 3$  folds, two subsets (A/B).
- ▶ Compute test error for each fold (1/2/3) and subset (A/B).

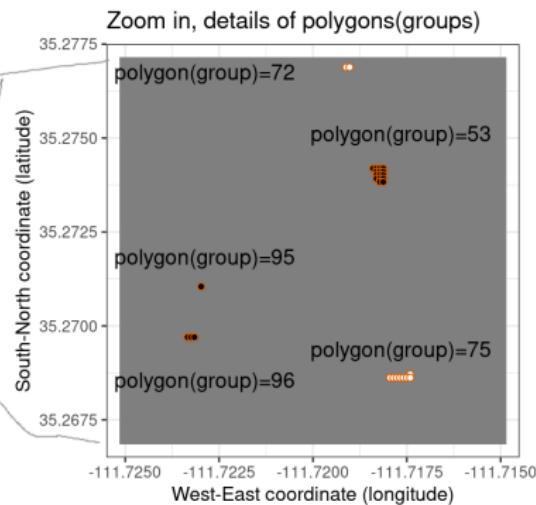
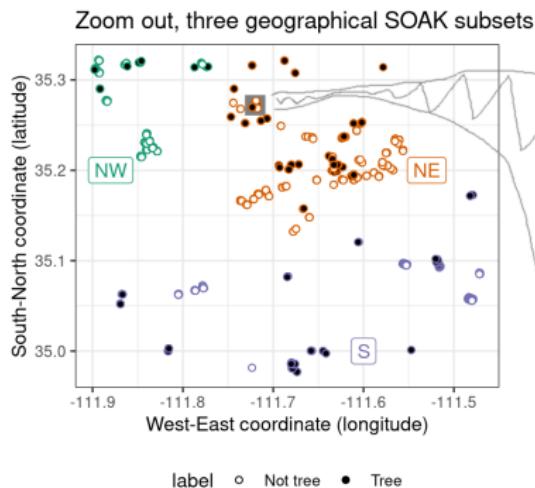


## Related work

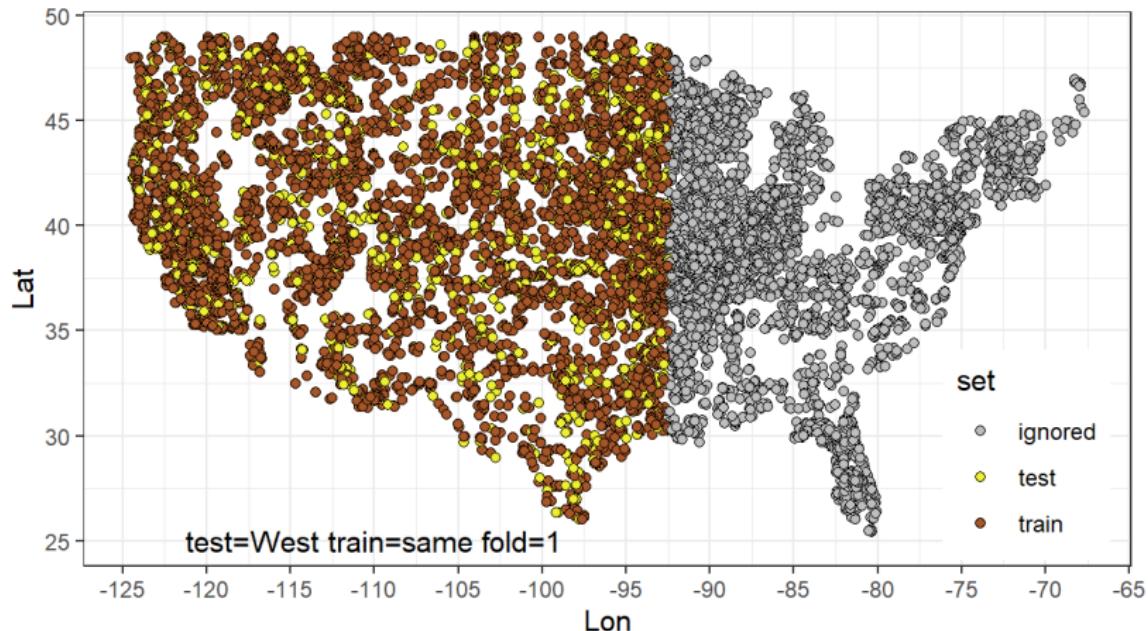
- ▶ Same/Other comparison has been used to evaluate **out-of-distribution predictions**, for example in computer vision, evaluating predictions on images with new position/rotation/scale values (Madan *et al.*, 2020).
- ▶ Farahani *et al.* (2021) review **domain adaptation** algorithms, and refer to the Other model as “unsupervised domain adaptation” because there are no labels available in the target domain (comparison with Same is not often present).
- ▶ **Algorithmic bias/fairness** benchmark data have interesting demographic subsets that could be used in SOAK (for example gender, race, etc), but this literature does not often discuss details of how cross-validation is used (Savoldi *et al.*, 2021).
- ▶ **Spatial cross-validation** has been used in geographical data analysis, and can be viewed as the “Other” model in SOAK (Ploton *et al.*, 2020).

# Proposed SOAK algorithm new to ML frameworks

- ▶ ML frameworks like scikit-learn and mlr3 implement cross-validation with **groups** of samples that must stay together when splitting.
- ▶ For example (below), satellite image segmentation, trees vs background, Shenkin *et al.*: samples=pixels, grouped by polygon, SOAK subsets are geographical regions (NW, NE, S).
- ▶ SOAK: good predictions on one test **subset**, after training on Same/Other/All subsets? (can use together with groups)

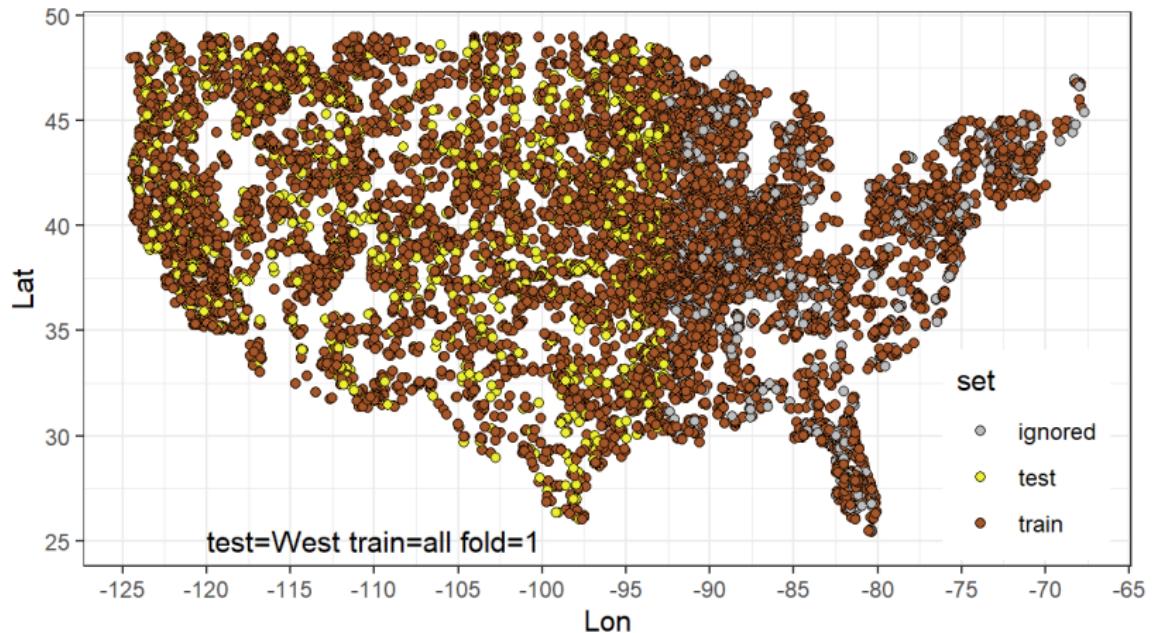


## Proposed SOAK algorithm (geographical data example)



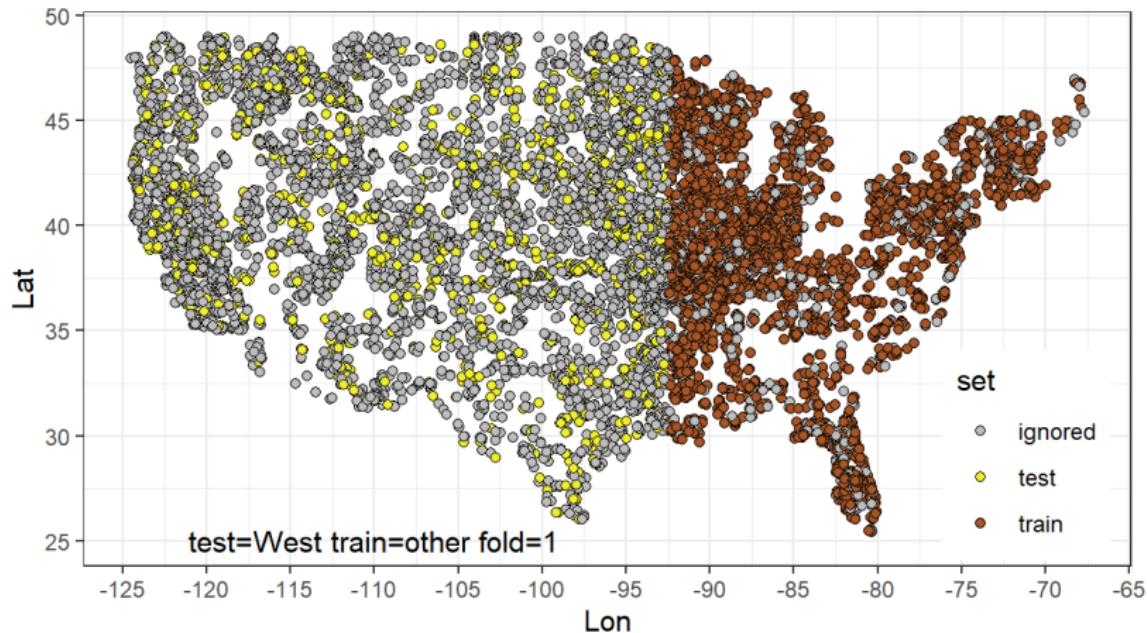
- ▶ Say we want good prediction in western USA.
- ▶ One of the K test sets is: subset=West and fold=1.
- ▶ Train on Same (West, fold $\neq$ 1) establishes a baseline.

## Proposed SOAK algorithm (geographical data example)



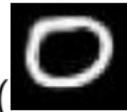
- ▶ Train on All (West+East,  $\text{fold} \neq 1$ ) would be less accurate than Same if subsets are different, and more accurate if subsets are similar (more relevant training data).

## Proposed SOAK algorithm (geographical data example)

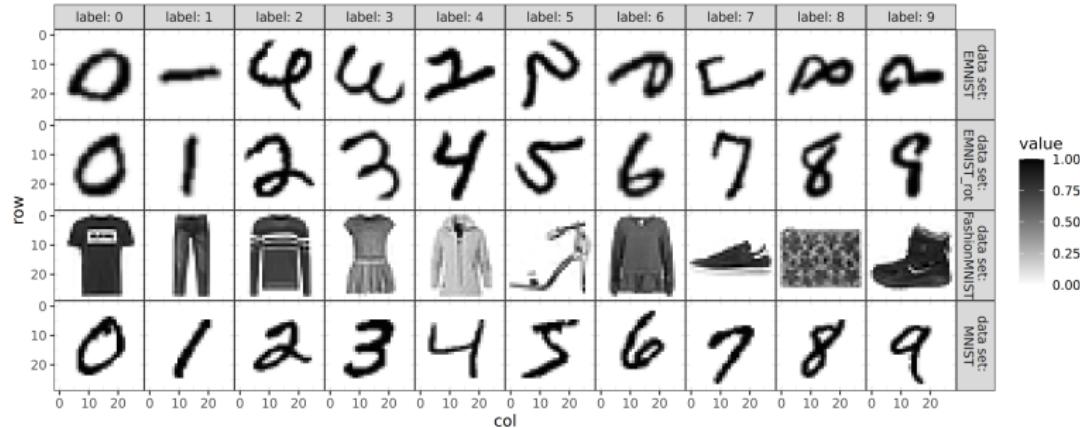


- ▶ Train on Other (East,  $\text{fold} \neq 1$ ) would be less accurate than Same if subsets are different.
- ▶ If subsets are similar, then the larger of Same and Other should be more accurate (more relevant training data).

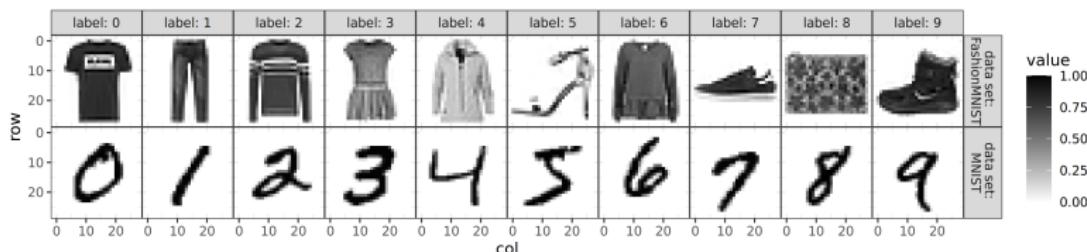
# ImagePair data: train on MNIST and accurately predict on MNIST variants?



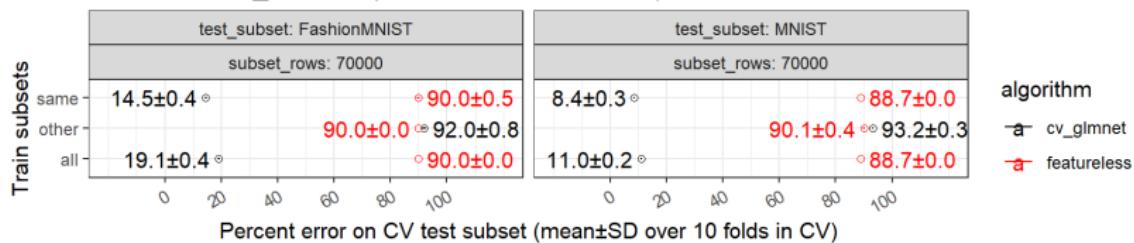
- ▶ Expect:  $g(\text{boot})$  and  $h(\text{circle})$  are not accurate.
- ▶ But train on MNIST, predict on EMNIST\_rot (upright digits) should be possible, right? (Vote!) Let's use SOAK to find out!
- ▶ Create three new IPair data sets by combining MNIST with variants: EMNIST, EMNIST\_rot, FashionMNIST.
- ▶ Each data set has two subsets: MNIST/variant.



# SOAK for IPair\_Fashion data set (MNIST+FashionMNIST)

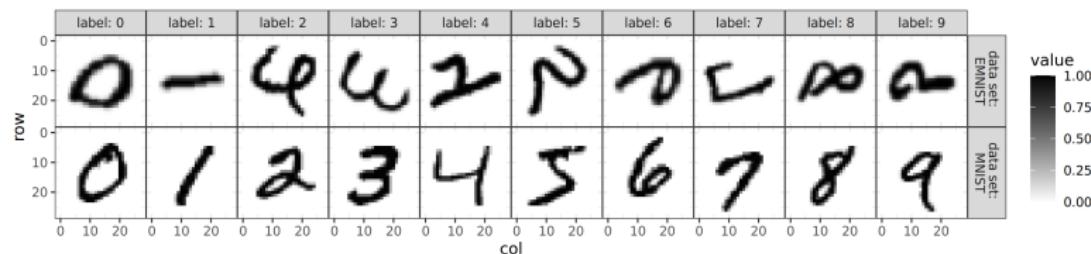


Data set: IPair\_Fashion (MNIST+FashionMNIST)

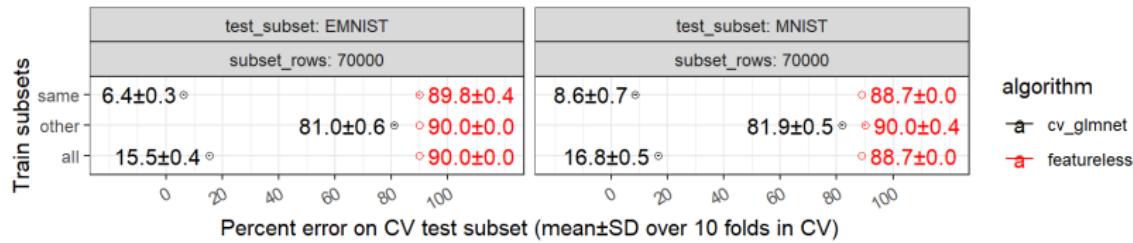


- ▶ **cv\_glmnet** is L1-regularized linear model.
- ▶ **featureless** baseline always predicts most frequent class.
- ▶ Other **cv\_glmnet** has greater test error than **featureless**.
- ▶ The patterns in the two subsets are too different for **Other cv\_glmnet** to learn anything useful for prediction. (expected)

# SOAK for IPair\_E data set (MNIST+EMNIST)

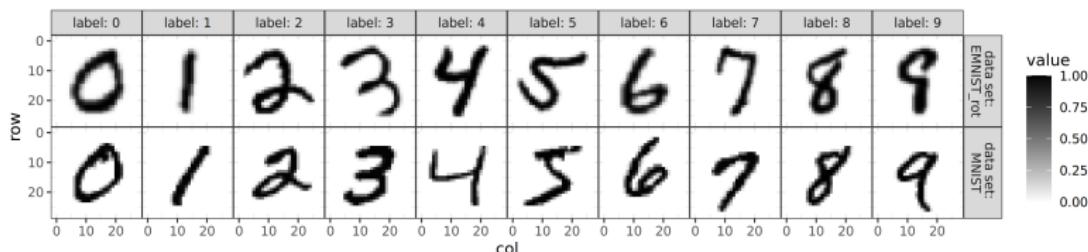


Data set: IPair\_E (MNIST+EMNIST)

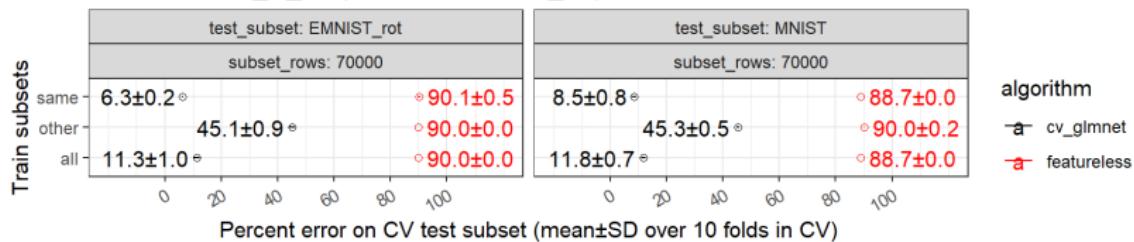


- ▶ **Other cv\_glmnet** has significantly smaller test error than **featureless**, so linear model learns something that useful for predicting on the other subset.
- ▶ But since **Other** error rate is much larger than **Same**, clearly the pattern is very different between MNIST/EMNIST.

# SOAK for IPair\_E\_rot data set (MNIST+EMNIST\_rot)



Data set: IPair\_E\_rot (MNIST+EMNIST\_rot)

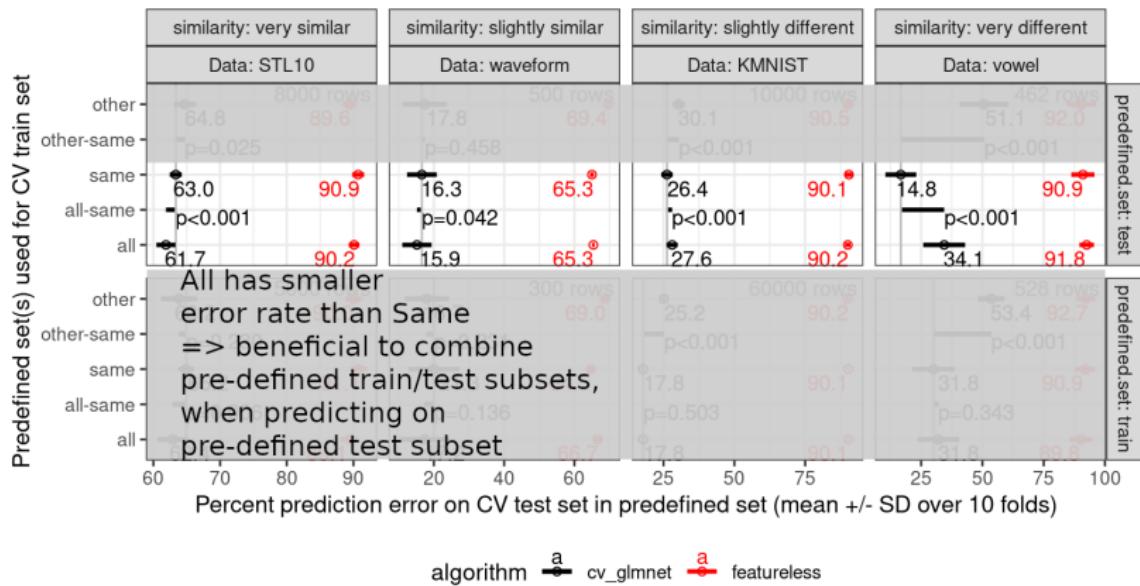


- ▶ **Other cv\_glmnet** has even smaller test error, indicating even more similarity between MNIST and EMNIST\_rot data sets.
- ▶ But **Other/All** test error are still not as small as **Same**.
- ▶ Significant difference between patterns learnable/predictable by linear model in MNIST/EMNIST\_rot. (surprising)

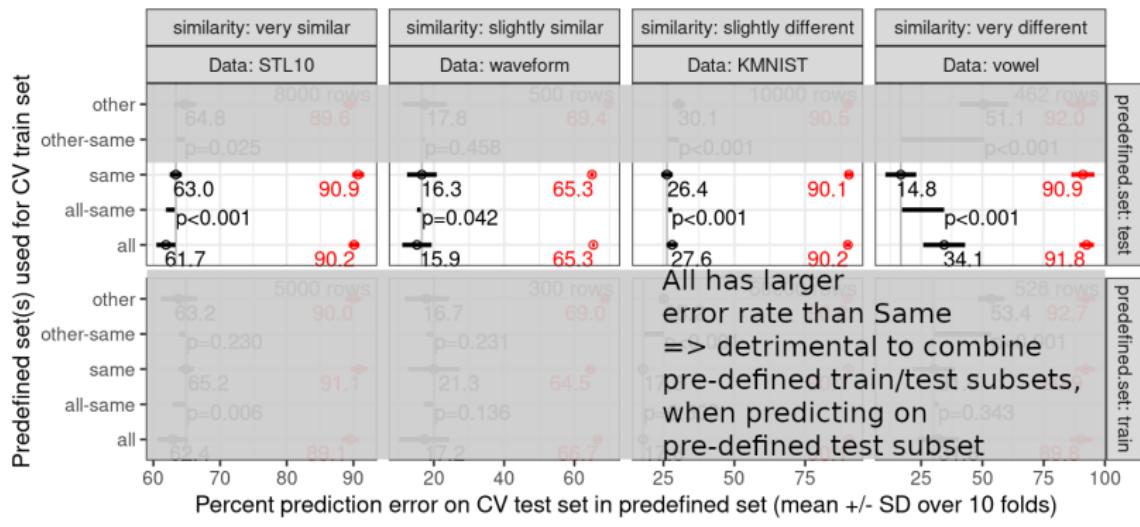
## Benchmark data with pre-defined train/test subsets

- ▶ Machine learning researchers evaluate new algorithms using benchmark data sets, which sometimes have pre-defined train/test subsets.
- ▶ For example KMNIST is an image classification data set with 60,000 images in a pre-defined train subset, and 10,000 images in a pre-defined test subset.
- ▶ STL10 is another image classification data set with 5000 images in a pre-defined train subset, and 8000 images in a pre-defined test subset.
- ▶ Are the learnable/predictable patterns in the pre-defined train/test subsets similar? (expected if random sampling was used to create pre-defined subsets)
- ▶ Use pre-defined train/test subsets in SOAK, to see if patterns are learnable/predictable across pre-defined subsets.

# Benchmark data with pre-defined train/test subsets

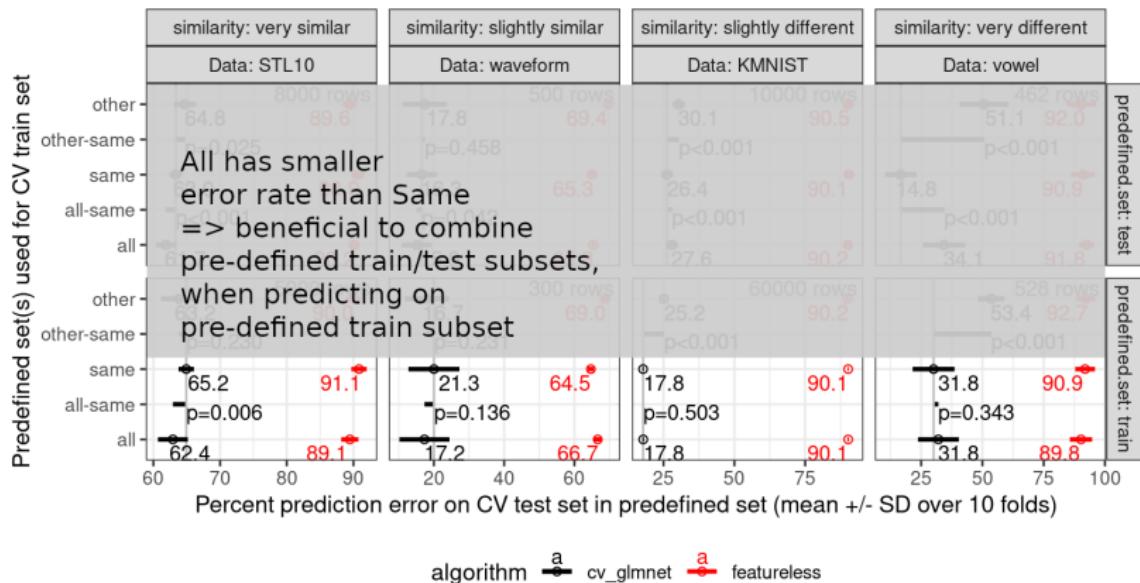


# Benchmark data with pre-defined train/test subsets

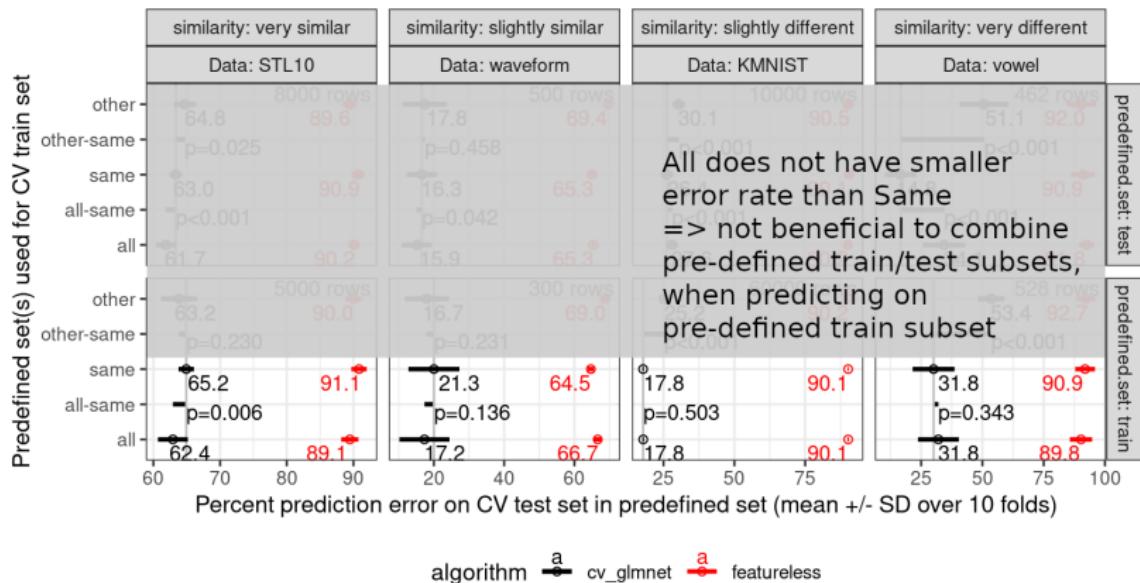


algorithm cv\_glmnet featureless

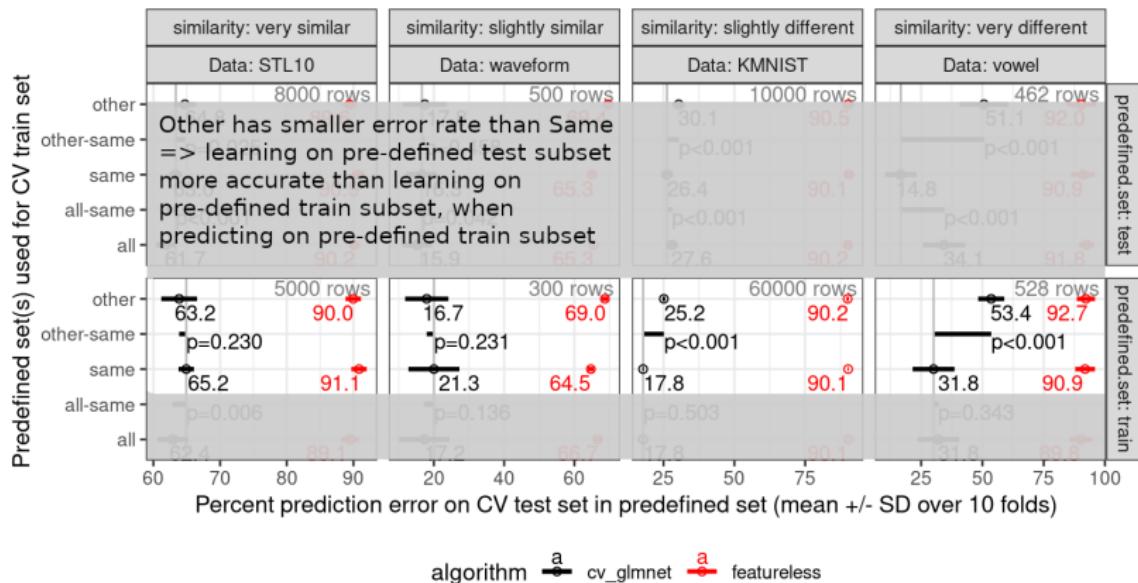
# Benchmark data with pre-defined train/test subsets



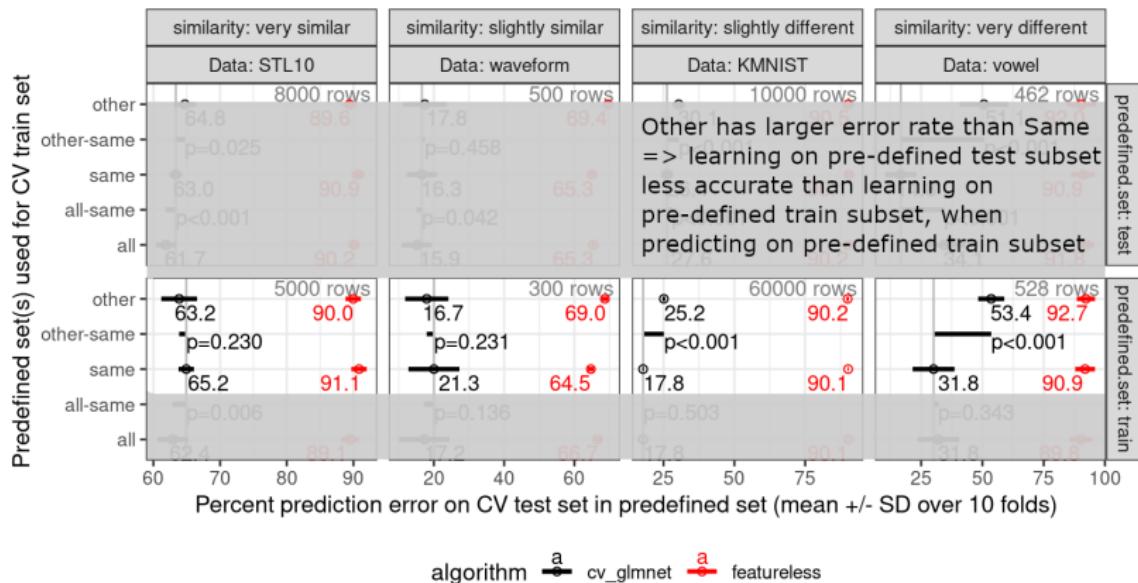
# Benchmark data with pre-defined train/test subsets



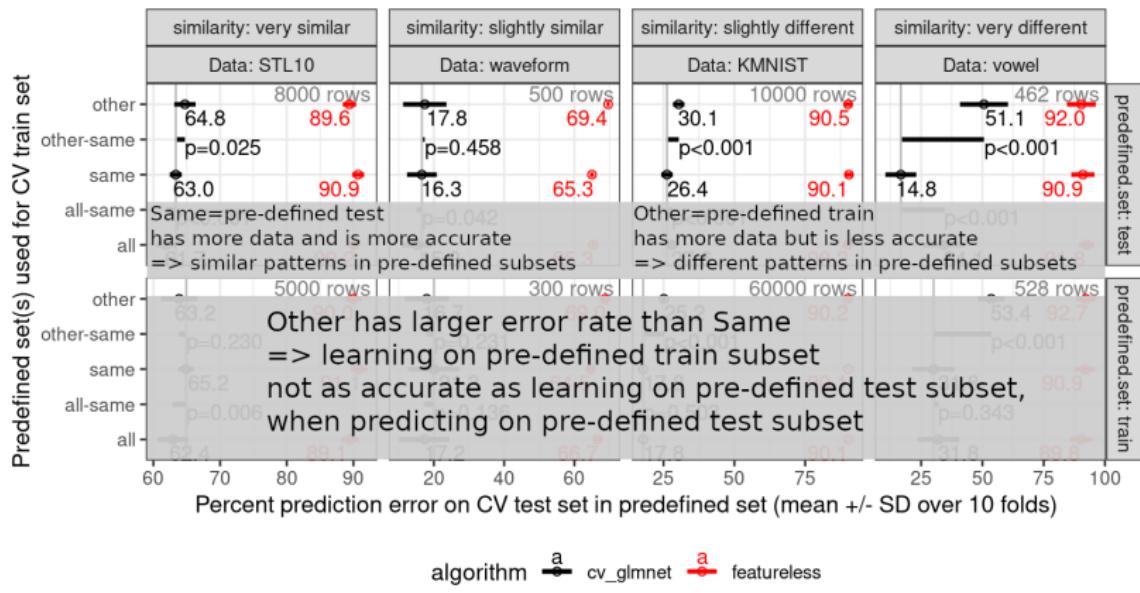
# Benchmark data with pre-defined train/test subsets



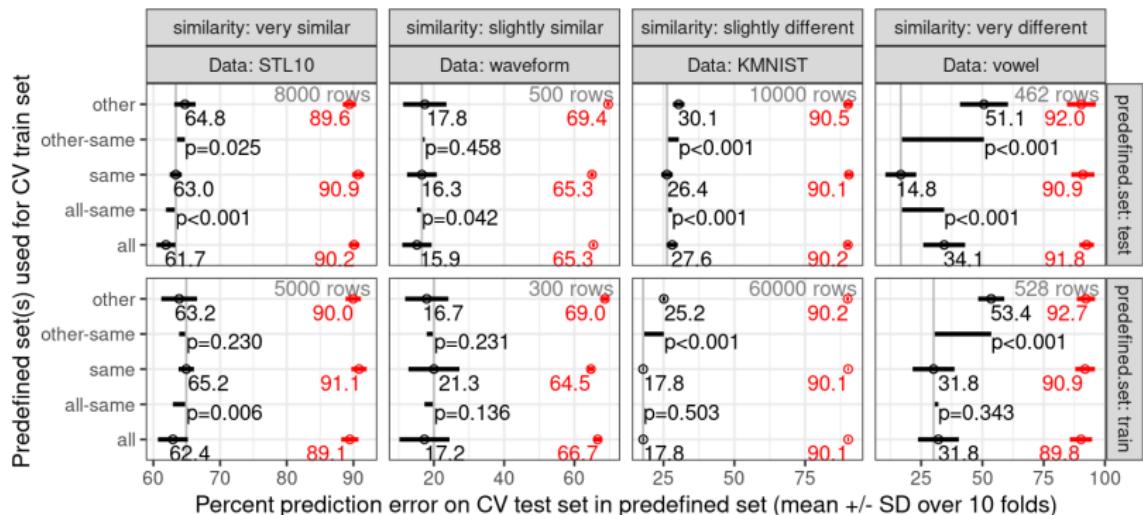
# Benchmark data with pre-defined train/test subsets



# Benchmark data with pre-defined train/test subsets



# Benchmark data with pre-defined train/test subsets



algorithm    cv\_glmnet    featureless

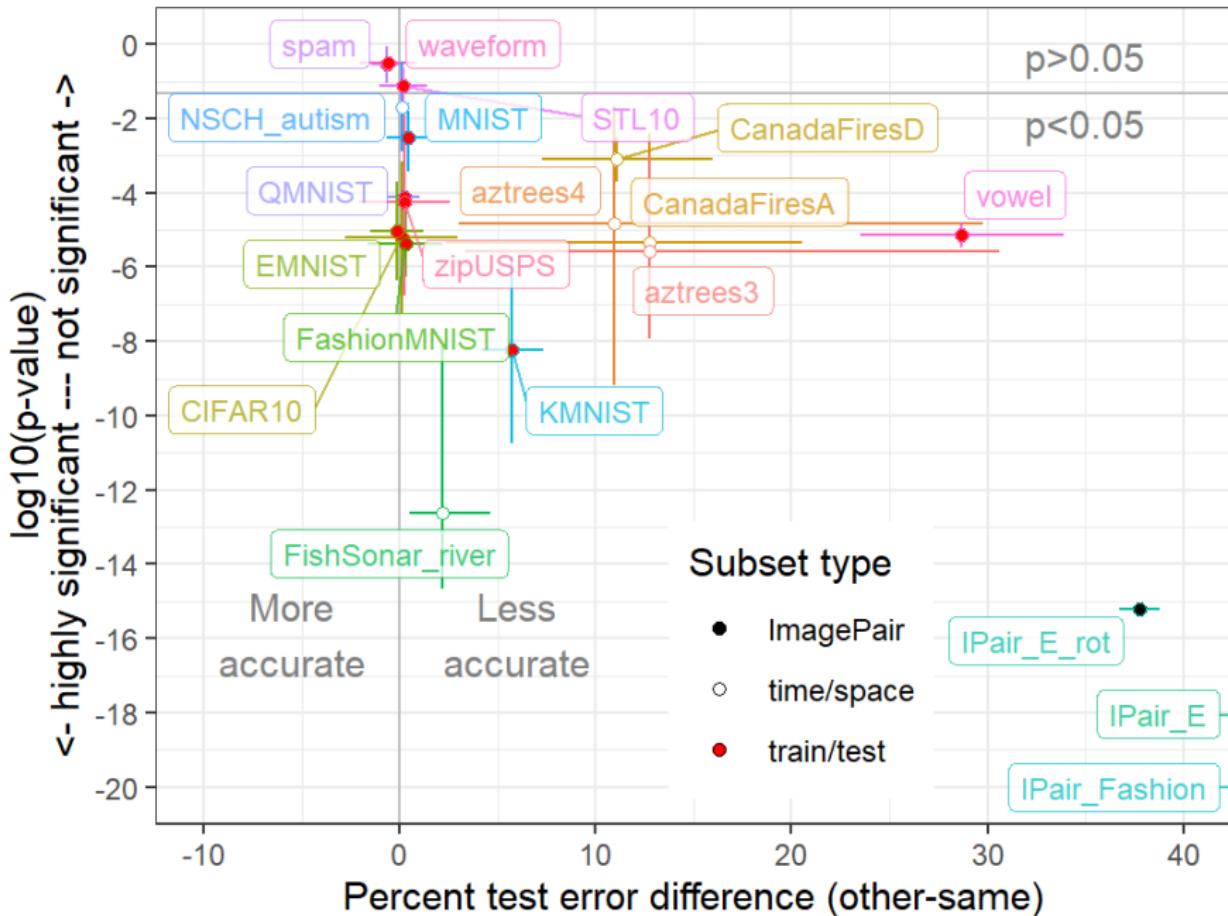
- ▶ Left data sets have similar pre-defined train/test subsets (expected), All error is always less than Same, and Other error is either greater or less than Same, depending on subset sizes.
- ▶ Right data sets have different pre-defined train/test subsets (surprising), All error is always greater than or equal to Same, and Other error is always greater than Same.

# 20 classification data sets analyzed using SOAK

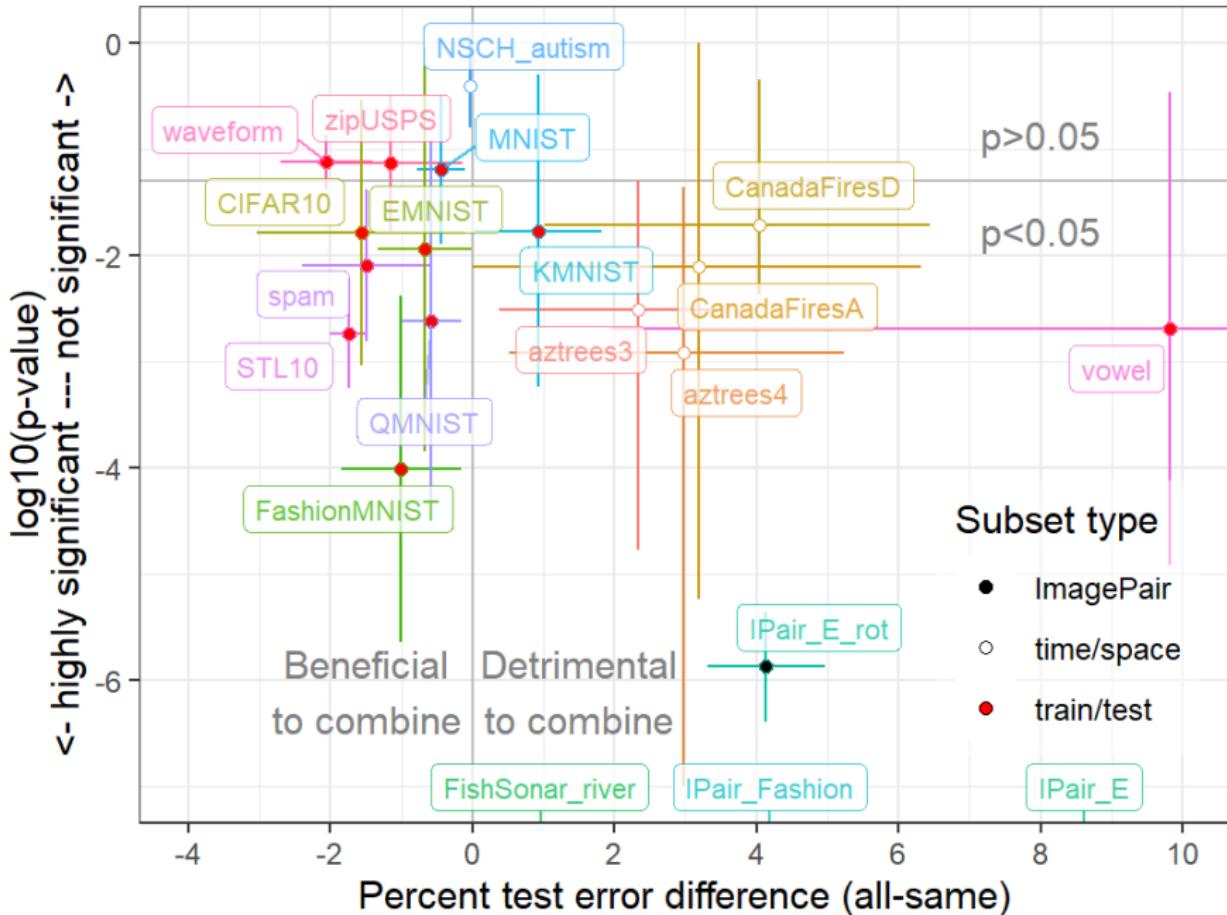
We considered MNIST and variants as subsets (**ImagePair**),  
data from collaborations (**time/space** subsets),  
and benchmark data with pre-defined **train/test** subsets.

| Type            | Data            | rows    | features | classes | subsets | imb. |
|-----------------|-----------------|---------|----------|---------|---------|------|
| 1 ● ImagePair   | IPair_E         | 140000  | 784      | 10      | 2       | 1.0  |
| 2 ● ImagePair   | IPair_E_rot     | 140000  | 784      | 10      | 2       | 1.0  |
| 3 ● ImagePair   | IPair_Fashion   | 140000  | 784      | 10      | 2       | 1.0  |
| 4 ○ time/space  | CanadaFiresA    | 4827    | 46       | 2       | 4       | 7.0  |
| 5 ○ time/space  | CanadaFiresD    | 1491    | 46       | 2       | 4       | 1.6  |
| 6 ○ time/space  | FishSonar_river | 2815744 | 81       | 2       | 4       | 1.2  |
| 7 ○ time/space  | NSCH_autism     | 46010   | 364      | 2       | 2       | 1.5  |
| 8 ○ time/space  | aztrees3        | 5956    | 21       | 2       | 3       | 2.0  |
| 9 ○ time/space  | aztrees4        | 5956    | 21       | 2       | 4       | 4.9  |
| 10 ● train/test | CIFAR10         | 60000   | 3072     | 10      | 2       | 5.0  |
| 11 ● train/test | EMNIST          | 70000   | 784      | 10      | 2       | 6.0  |
| 12 ● train/test | FashionMNIST    | 70000   | 784      | 10      | 2       | 6.0  |
| 13 ● train/test | KMNIST          | 70000   | 784      | 10      | 2       | 6.0  |
| 14 ● train/test | MNIST           | 70000   | 784      | 10      | 2       | 6.0  |
| 15 ● train/test | QMNIST          | 120000  | 784      | 10      | 2       | 1.0  |
| 16 ● train/test | STL10           | 13000   | 27648    | 10      | 2       | 1.6  |
| 17 ● train/test | spam            | 4601    | 57       | 2       | 2       | 2.0  |
| 18 ● train/test | vowel           | 990     | 10       | 11      | 2       | 1.1  |
| 19 ● train/test | waveform        | 800     | 21       | 3       | 2       | 1.7  |
| 20 ● train/test | zipUSPS         | 9298    | 256      | 10      | 2       | 3.6  |

# Accurate prediction on a new subset?



# Is it beneficial to combine subsets?



## Summary of contributions

- ▶ Proposed SOAK algorithm estimates similarity of learnable patterns between subsets (space, time, etc).
- ▶ SOAK idea is new to ML frameworks (proposed **subset** column/idea not the same as **group/stratum**).
- ▶ Free/open-source R package available in mlr3 framework (easy parallelization over algorithms, data sets, train/test splits) <https://github.com/tdhock/mlr3resampling>
- ▶ Ran SOAK in parallel over 20 classification data sets, 10 folds, 2–4 subsets, Same/Other/All (1200+ train/test splits).
- ▶ Train on MNIST, predict on FashionMNIST (impossible), predict on EMNIST (surprisingly difficult, both are digits).
- ▶ Most pre-defined train/test subsets in benchmark data are similar (STL10/waveform), some are not (KMNIST/vowel).
- ▶ We observed similarity between years in Autism data (slight benefit to combining years, predicting on new year works).
- ▶ In fires/trees/fish data, we observed significant differences between images/regions/rivers.

Introduction: two common questions in collaborations involving scientific applications of machine learning

Train on one subset and accurately predict on another?

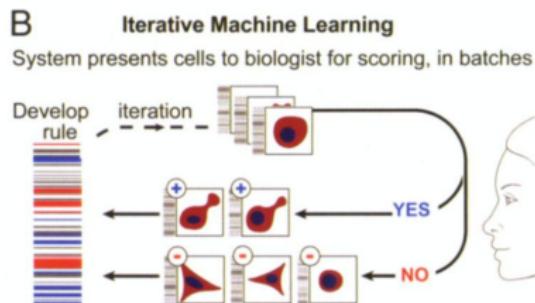
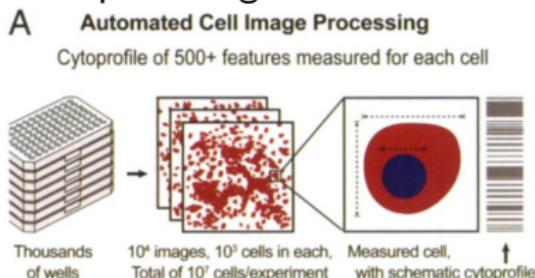
SOAK: Same/Other/All K-fold cross-validation for estimating similarity of patterns in data subsets (arXiv:2410.08643)

How to deal with class imbalance?

AUM: Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization (JMLR'23)

# Review of supervised binary classification

- ▶ Given pairs of inputs  $\mathbf{x} \in \mathbb{R}^P$  and outputs  $y \in \{0, 1\}$  can we learn a score  $f(\mathbf{x}) \in \mathbb{R}$ , predict  $y = 1$  when  $f(\mathbf{x}) > 0$ ?
- ▶ Example: email,  $\mathbf{x}$  = bag of words,  $y$  = spam or not.
- ▶ Example: images. Jones *et al.* PNAS 2009.

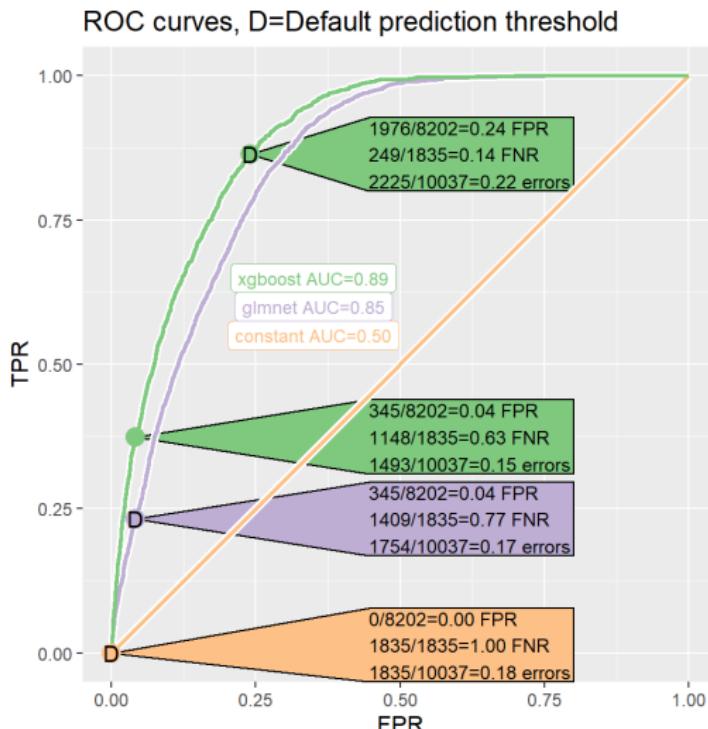


Gradient descent algorithms (Logistic regression, SVM, etc) minimize a differentiable surrogate of zero-one loss = sum of:

**False positives:**  $f(\mathbf{x}) > 0$  but  $y = 0$  (predict budding, but cell is not).

**False negatives:**  $f(\mathbf{x}) < 0$  but  $y = 1$  (predict not budding, but cell is).

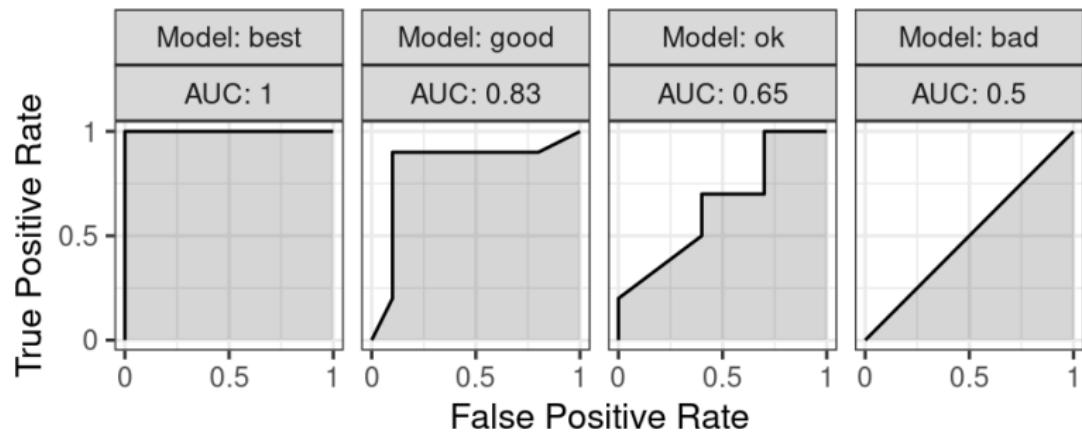
# ROC curves: fair comparison with different default FPR



- ▶ Imbalanced labels: 18% positive, 82% negative.
- ▶ At defaults (D), glmnet has fewer errors (misleading).
- ▶ At FPR=4%, xgboost has fewer errors (fair comparison).

# Receiver Operating Characteristic (ROC) Curves

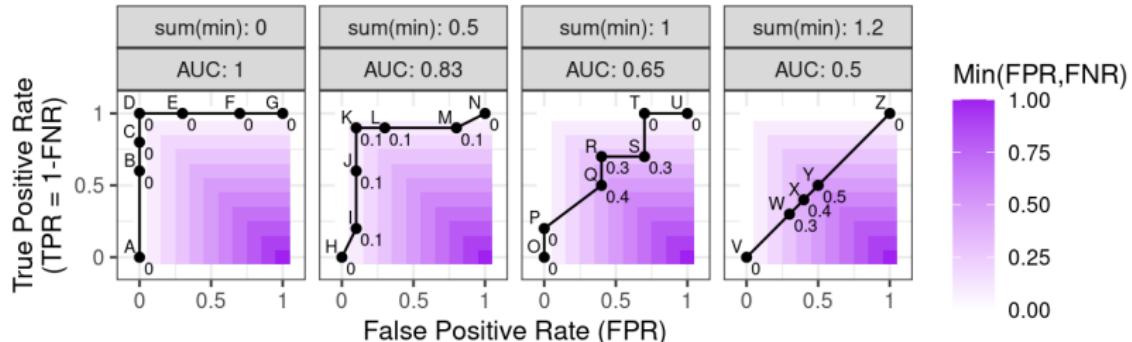
- ▶ Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- ▶ ROC curve of learned  $f$  is plot of True Positive Rate vs False Positive Rate: each point on the ROC curve is a different constant  $c \in \mathbb{R}$  added to the predicted values:  $f(\mathbf{x}) + c$ .
- ▶  $c = \infty$  means always predict positive label ( $\text{FPR}=\text{TPR}=1$ ).
- ▶  $c = -\infty$  means always predict negative label ( $\text{FPR}=\text{TPR}=0$ ).
- ▶ Best classifier has a point near upper left ( $\text{TPR}=1$ ,  $\text{FPR}=0$ ), with large Area Under the Curve (AUC).



## Research question and new idea

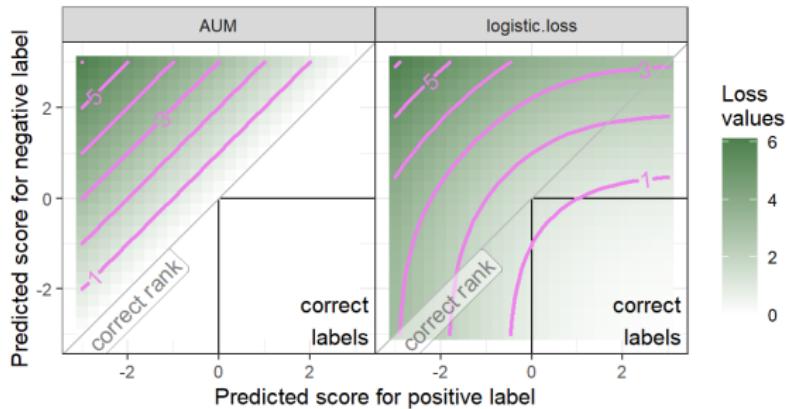
Can we learn a binary classification function  $f$  which directly optimizes the ROC curve?

- ▶ Most algorithms involve minimizing a differentiable surrogate of the zero-one loss, which is not the same.
- ▶ The Area Under the ROC Curve (AUC) is piecewise constant (gradient zero almost everywhere), so can not be used with gradient descent algorithms.
- ▶ We proposed (Hocking, Hillman 2023) to encourage points to be in the upper left of ROC space, using a loss function which is a differentiable surrogate of the sum of  $\min(\text{FPR}, \text{FNR})$ .

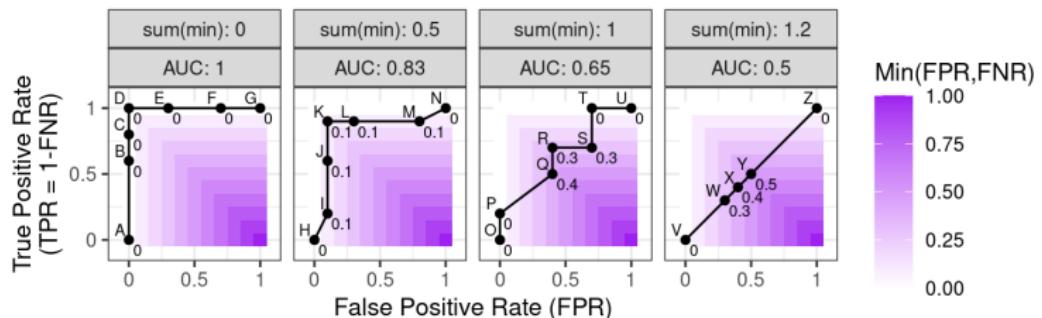


# Comparing proposed loss with baselines

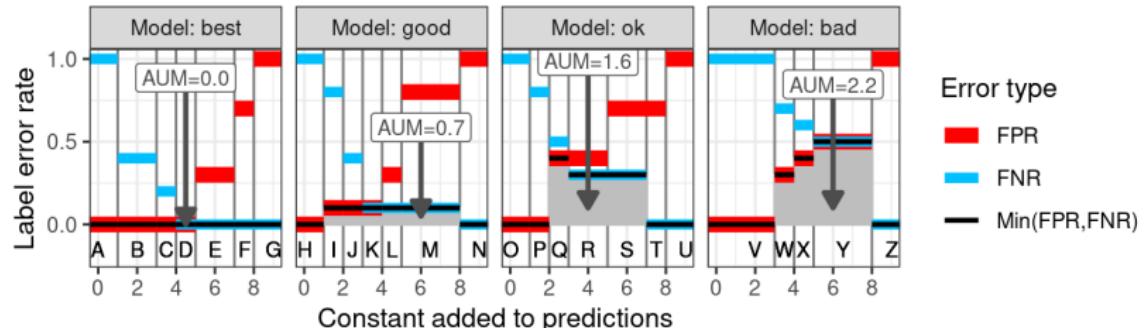
- ▶ Classic baselines: hinge and logistic loss, sum over samples,  $\ell[yf(x)]$ .
- ▶ Bamber (1975) proved ROC-AUC relation to Mann-Whitney U statistic (double sum over all pairs of positive and negative samples).
- ▶ Recently: SVM<sup>struct</sup> (Joachims 2005), X-risk (Yang 2022), All Pairs Squared Hinge (Rust and Hocking 2023), sum loss over pairs of positive and negative samples,  $\ell[f(x^+) - f(x^-)]$ .
- ▶ Proposed: sort-based AUM loss (sum over points on ROC curve).
- ▶ Figure below: loss for two samples: one positive, one negative.



# Large AUC $\approx$ small Area Under Min(FP,FN) (AUM)

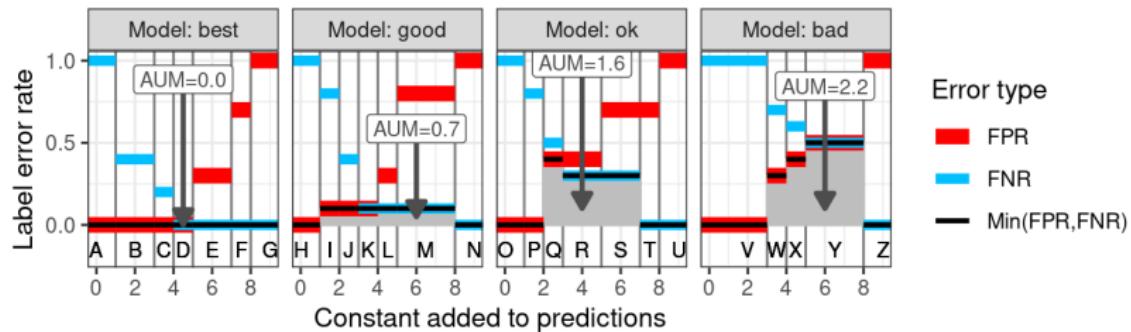


Above: purple heat map = numbers near dots = distance to top or left  
= same as black min error rate functions below.



Hocking, Hillman, *Journal of Machine Learning Research* (2023).

# Computing Sum of Min (SM) over all ROC points

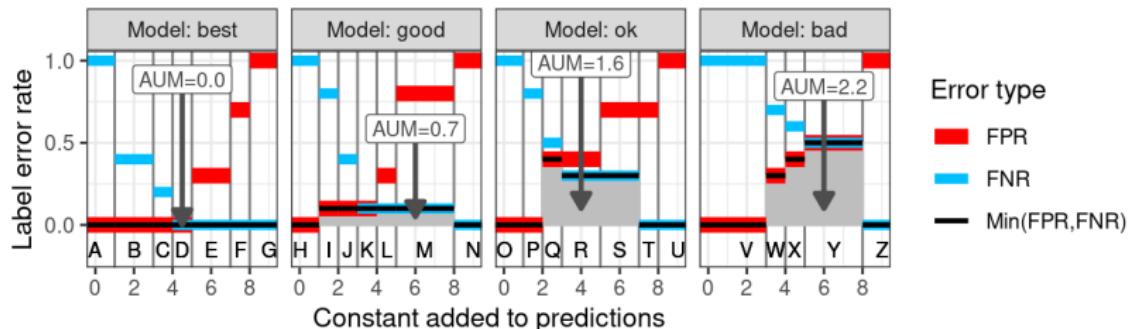


- ▶ For  $N$  samples, there are  $\leq N + 1$  points on the ROC curve,
- ▶ with sorted thresholds of  $c$ ,  $T_1 \leq \dots \leq T_N \in \mathbb{R}$  (grey lines),
- ▶ and corresponding min error values  $M_2, \dots, M_N$  (black).
- ▶ Then if  $I$  is the indicator function, we can write the sum of the min (SM), over all ROC points, as:

$$\text{SM} = \sum_{i=2}^N I[T_i \neq T_{i-1}] M_i = \sum_{i: T_i \neq T_{i-1}} M_i.$$

( $\neq$  required: a tie  $T_i = T_{i-1}$  deletes a point from the ROC curve)

# Computing proposed loss, Area Under Min (AUM)



The proposed AUM can be interpreted as an L1 relaxation of SM,

$$(\text{gradient zero}) \text{ SM} = \sum_{i=2}^N \underbrace{I[T_i \neq T_{i-1}]}_{L_0} M_i = \sum_{i: T_i \neq T_{i-1}} M_i.$$

$$(\text{gradient non-zero}) \text{ AUM} = \sum_{i=2}^N \underbrace{[T_i - T_{i-1}]}_{L_1} M_i.$$

AUM is therefore a surrogate loss for ROC-SM minimization.  
L1 relaxation  $\Rightarrow$  constant/non-zero gradients.

## ROC curve pytorch code uses argsort

```
def ROC_curve(pred_tensor, label_tensor):
    sorted_indices = torch.argsort(-pred_tensor)
    ... # torch.cumsum() etc
    return { # a dictionary of torch tensors
        "FPR":FPR, "FNR":FNR, "TPR":1 - FNR,
        "min(FPR,FNR)":torch.minimum(FPR, FNR),
        "min_constant":torch.cat([
            torch.tensor([-torch.inf]), uniq_thresh]),
        "max_constant":torch.cat([
            uniq_thresh, torch.tensor([torch.inf])]) }
>>> pd.DataFrame(ROC_curve(torch.tensor(
...     [2.0, -3.5, -1.0, 1.5]), torch.tensor([0,0,1,1])))
   FPR  FNR  TPR  min(FPR,FNR)  min_constant  max_constant
0  0.0  1.0  0.0          0.0           -inf         -2.0
1  0.5  1.0  0.0          0.5          -2.0         -1.5
2  0.5  0.5  0.5          0.5          -1.5          1.0
3  0.5  0.0  1.0          0.0           1.0          3.5
4  1.0  0.0  1.0          0.0           3.5           inf
```

## AUC and proposed AUM both use ROC curve

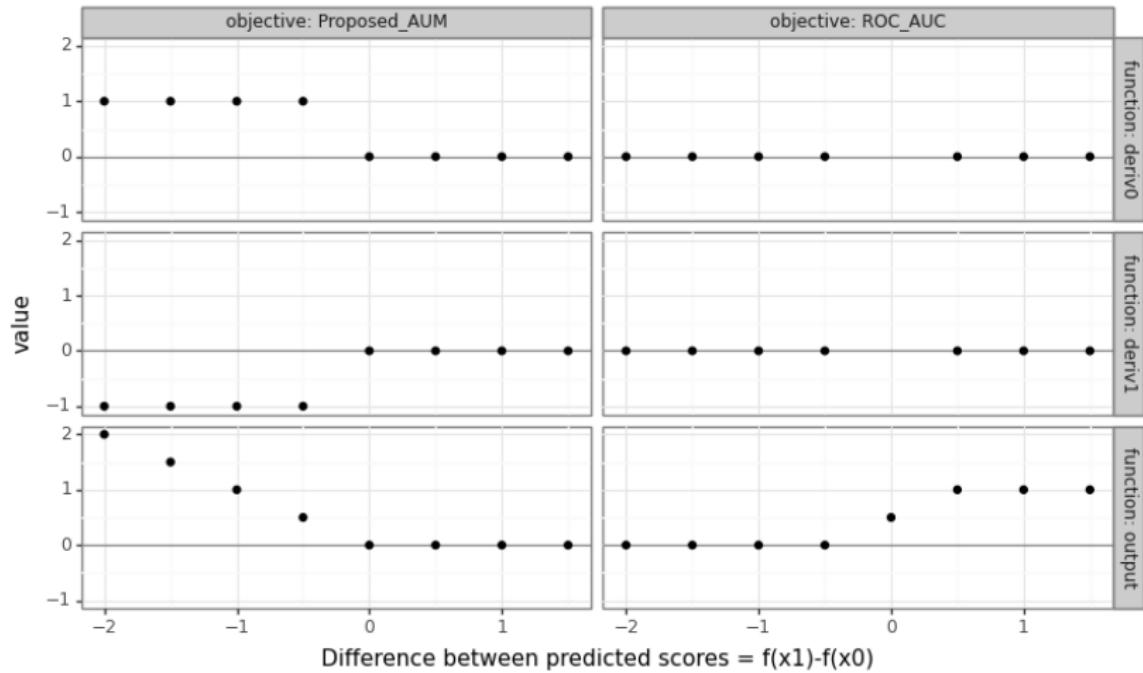
```
def ROC_AUC(pred_tensor, label_tensor):
    "Classic metric, but gradient zero almost everywhere"
    roc = ROC_curve(pred_tensor, label_tensor)
    FPR_diff = roc["FPR"][1:]-roc["FPR"][:-1]
    TPR_sum = roc["TPR"][1:]+roc["TPR"][:-1]
    return torch.sum(FPR_diff*TPR_sum/2.0)

def Proposed_AUM(pred_tensor, label_tensor):
    "Surrogate loss, non-zero gradient for predictions"
    roc = ROC_curve(pred_tensor, label_tensor)
    min_FPR_FNR = roc["min(FPR,FNR)"][1:-1]
    constant_diff = roc["min_constant"][1:].diff()
    return torch.sum(min_FPR_FNR * constant_diff)
```

<https://tdhock.github.io/blog/2024/torch-roc-aum/>

# Proposed AUM pytorch code, auto-grad demo

- ▶ Assume two samples,  $(x_0, y_0 = 0), (x_1, y_1 = 1)$ ,
- ▶ Plot objective and gradient with respect to predicted scores.



## ROC curve R torch code uses argsort

```
ROC_curve <- function(pred_tensor, label_tensor){  
  sorted_indices = torch_argsort(-pred_tensor$flatten())  
  ... # $cumsum() $diff() etc.  
  list(FPR=FPR, FNR=FNR, TPR=1 - FNR,  
       "min(FPR,FNR)"=torch_minimum(FPR, FNR),  
       min_constant=torch_cat(c(torch_tensor(-Inf), uniq_thresh)),  
       max_constant=torch_cat(c(uniq_thresh, torch_tensor(Inf))))  
}  
> L <- ROC_curve(torch_tensor(c(2,-3.5,-1,1.5)),  
+                  torch_tensor(c(0, 0, 1, 1)))  
> data.frame(lapply(L, torch::as_array), check.names=FALSE)  
  FPR FNR TPR min.FPR.FNR. min_constant max_constant  
1 0.0 1.0 0.0          0.0        -Inf        -2.0  
2 0.5 1.0 0.0          0.5        -2.0        -1.5  
3 0.5 0.5 0.5          0.5        -1.5         1.0  
4 0.5 0.0 1.0          0.0         1.0         3.5  
5 1.0 0.0 1.0          0.0         3.5         Inf
```

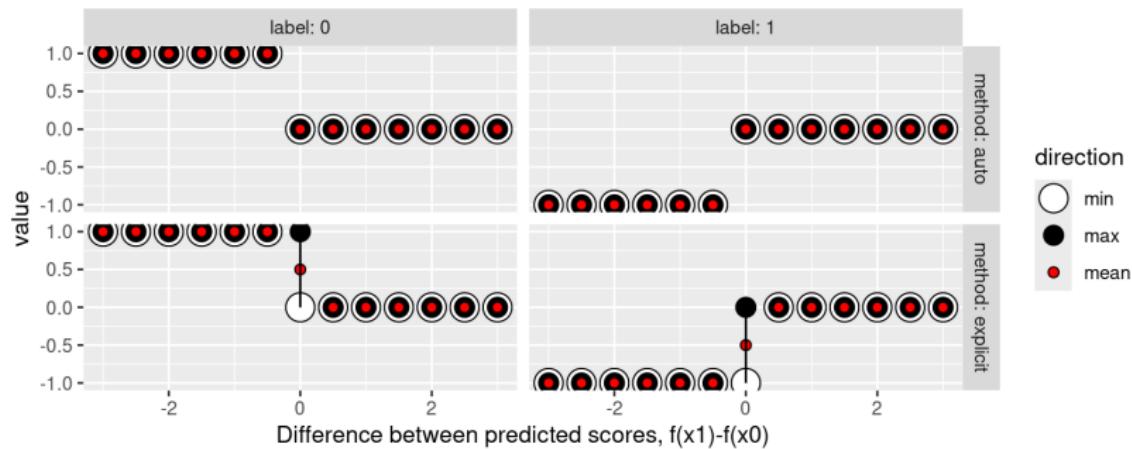
## R code for AUC and proposed AUM both use ROC curve

```
ROC_AUC <- function(pred_tensor, label_tensor){  
  roc = ROC_curve(pred_tensor, label_tensor)  
  FPR_diff = roc$FPR[2:N]-roc$FPR[1:-2]  
  TPR_sum = roc$TPR[2:N]+roc$TPR[1:-2]  
  torch_sum(FPR_diff*TPR_sum/2.0)  
}  
  
Proposed_AUM <- function(pred_tensor, label_tensor){  
  roc = ROC_curve(pred_tensor, label_tensor)  
  min_FPR_FNR = roc[["min(FPR,FNR)"]][2:-2]  
  constant_diff = roc$min_constant[2:N]$diff()  
  torch_sum(min_FPR_FNR * constant_diff)  
}
```

<https://tdhock.github.io/blog/2024/auto-grad-overhead/>

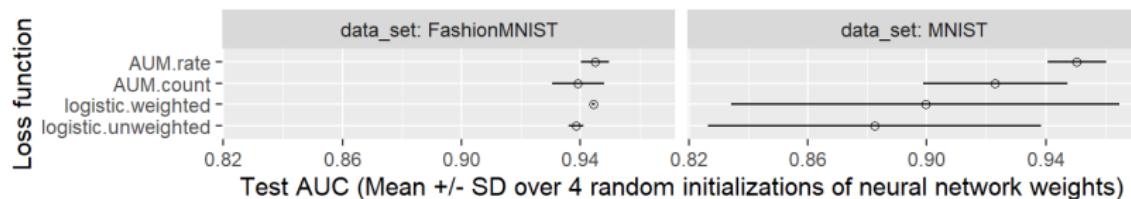
# Proposed AUM R torch code, auto-grad demo

- ▶ Assume two samples,  $(x_0, y_0 = 0), (x_1, y_1 = 1)$ ,
- ▶ Plot objective and gradient with respect to predicted scores.
- ▶ Compare explicit gradient with auto-grad from torch.



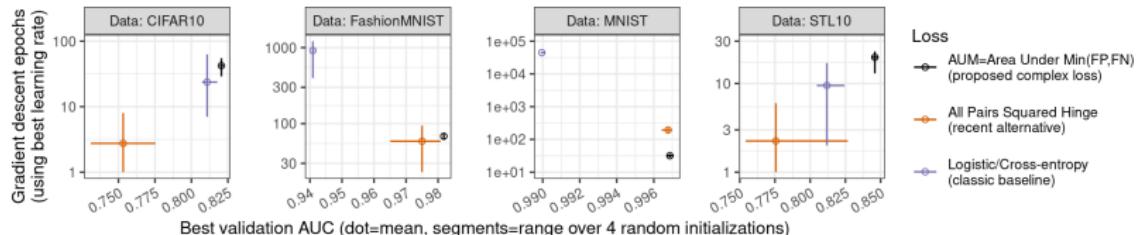
<https://tdhock.github.io/blog/2024/auto-grad-overhead/>

# Comparing proposed AUM with weighted logistic loss



- ▶ Image classification data sets (0–4=negative, 5–9 positive).
- ▶ Train set 1% positive, test set balanced.
- ▶ LeNet5 convolutional neural network, batch size 1000.
- ▶ Step size from  $10^{-4}$  to  $10^2$  (keep best).
- ▶ AUM rate uses Area Under Min of FPR/FNR, more accurate in these data than AUM count (FP/FN totals).
- ▶ logistic unweighted is usual binary cross-entropy loss (uniform weight=1 for each sample).
- ▶ for logistic weighted, we compute class frequencies,  $n_1 = \sum_{i=1}^N I[y_i = 1]$  and  $n_0$  similar; then weights are  $w_i = 1/n_{y_i}$  so that total weight of positive class equals total weight of negative class (more accurate in these data).

# AUM gradient descent increases validation AUC, four image classification data sets



- ▶ Unbalanced binary classification: 10% negative, 90% positive.
- ▶ Gradient descent with constant step size, best of  $10^{-4}$  to  $10^5$ .
- ▶ Full gradient (batch size = number of samples).
- ▶ Linear model, max iterations = 100,000.
- ▶ Max Validation AUC comparable or better than baselines: logistic loss and all paired squared hinge.
- ▶ Number of epochs comparable to baselines.
- ▶ AUM time per epoch is  $O(N \log N)$  (sort), small log factor larger than standard logistic/cross-entropy loss,  $O(N)$ .

## Discussion and future work

- ▶ Classic classification losses are L1 relaxations of the zero-one loss, defined as a sum over samples.
- ▶ Proposed AUM loss is an L1 relaxation defined as a sum over points on the ROC curve (requires sorting predicted scores).
- ▶ Proposed AUM loss can be used in gradient descent instead of logistic/binary cross-entropy loss. R/Python torch code!
- ▶ Best use with stochastic gradient algorithms? At least one positive and one negative example is required in each batch.
- ▶ Algorithms like SVM? (margin/kernel)
- ▶ How to adapt to multi-class setting, and other problems such as ranking/information retrieval?
- ▶ See our JMLR'23 paper for an application to supervised change-point detection, and arXiv:2410.08635 for an efficient line search that exploits the piecewise linear/constant nature of AUM/AUC.

Thanks! Please email me if you are interested to collaborate:  
toby.dylan.hocking@usherbrooke.ca



Reproducible slide/figure source code:

<https://github.com/tdhock/cv-same-other-paper>

<https://github.com/tdhock/max-generalized-auc>

# 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).

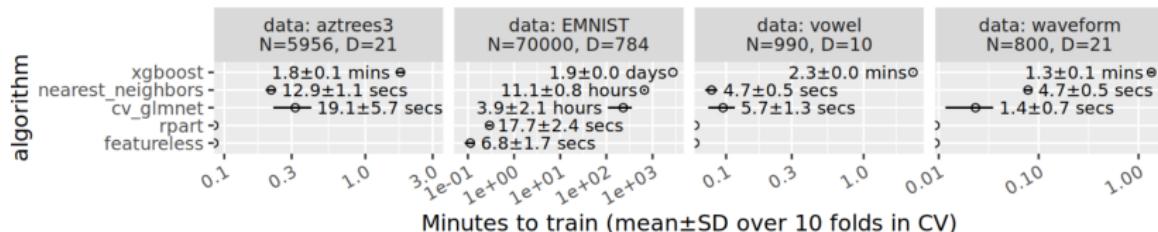
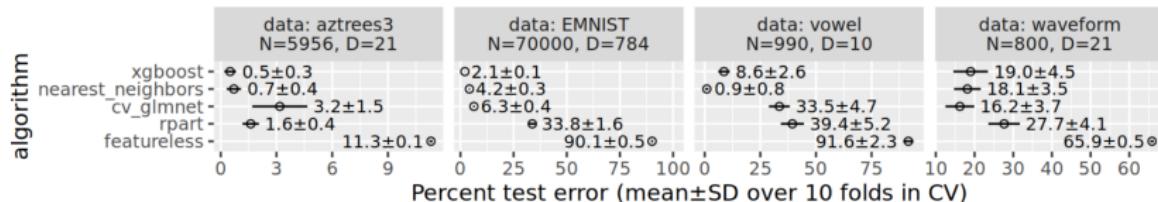
`nearest_neighbors` classic non-linear algorithm, as implemented in `kknn` R package. Schliep and Hechenbichler (2016).

`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.

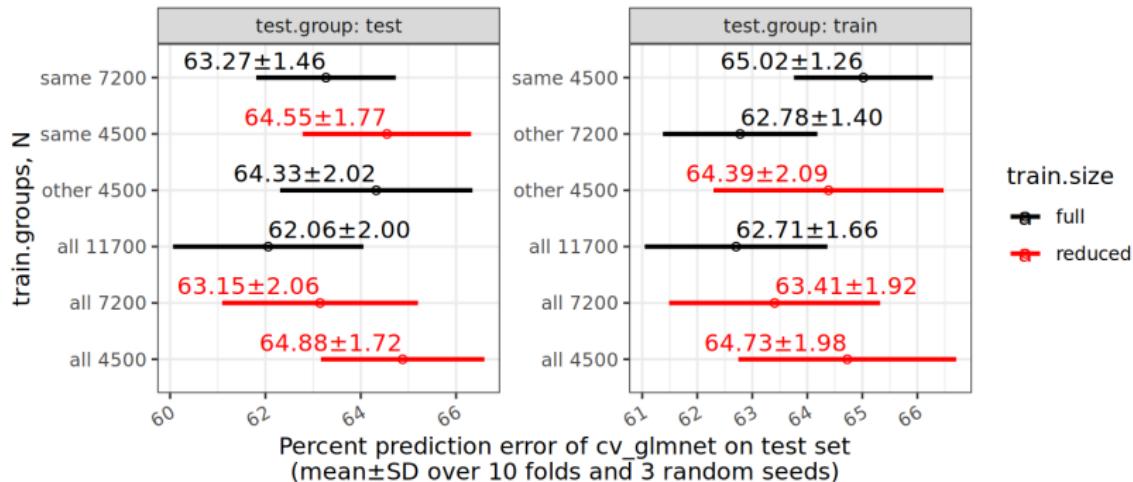
# Learning algorithms have different accuracy and speed

- ▶ Image segmentation/classification, and audio classification data sets.
- ▶ xgboost is slowest to train on all four data sets, most accurate in aztrees3, EMNIST.
- ▶ Other algorithms are faster and more accurate in vowel, waveform.
- ▶ Need to try a variety of algorithms for optimal prediction in any data.



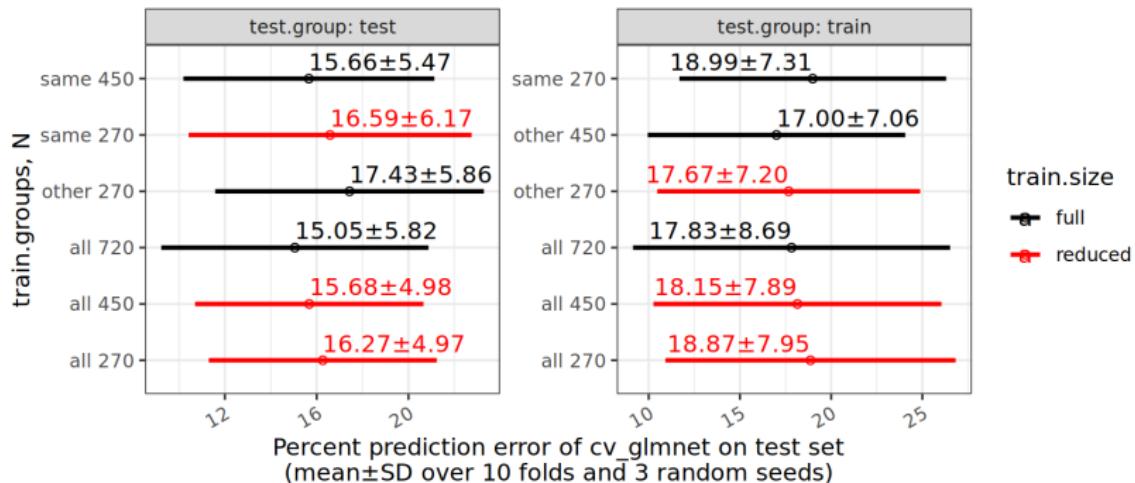
# Large sample size effect

Data set: STL10

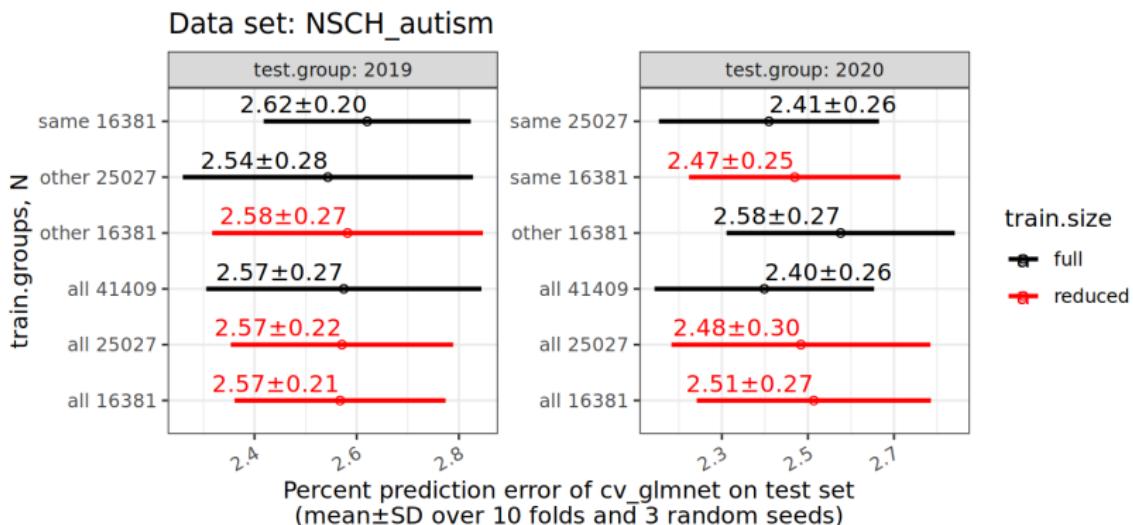


# Moderate sample size effect

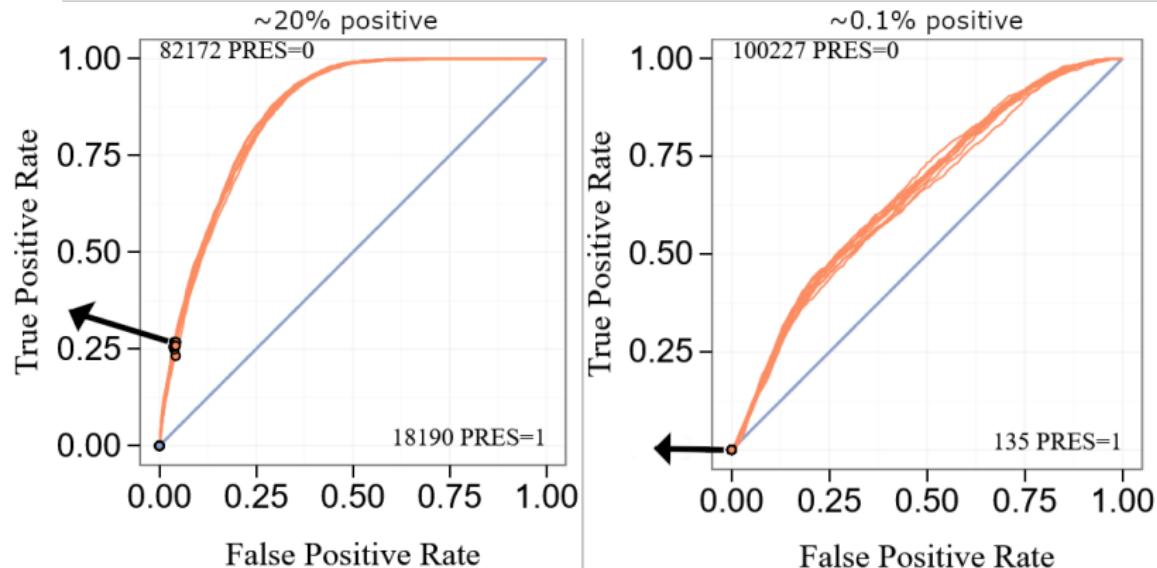
Data set: waveform



# Small sample size effect

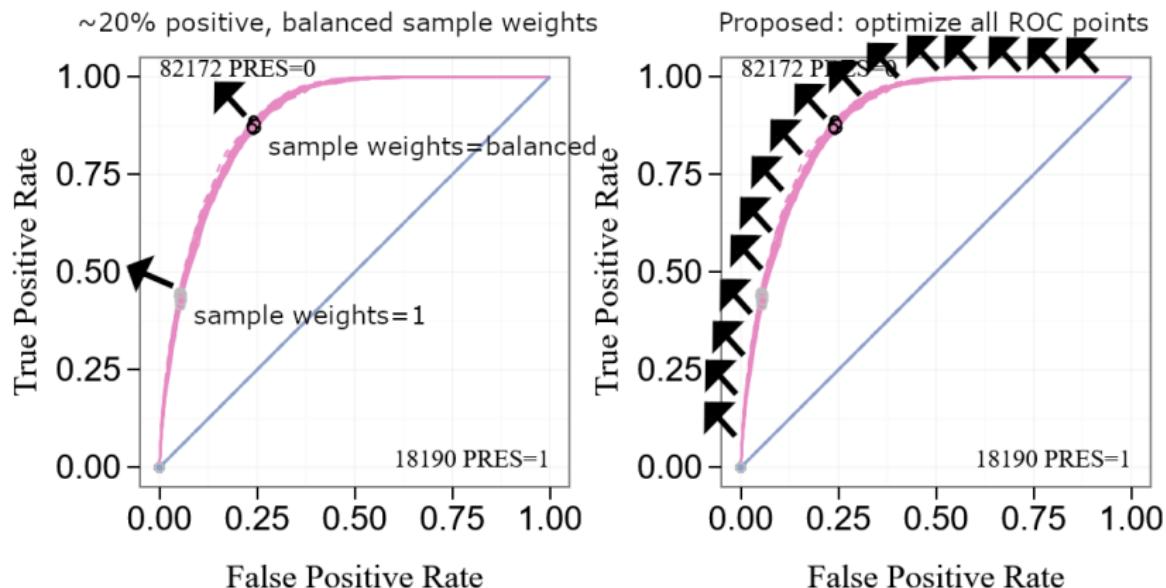


# Gradients of sample-based loss are influenced by imbalance



- ▶ Left: some imbalance, 20% positive labels, gradient 4x stronger along X axis / False Positive Rate.
- ▶ Right: large imbalance, 0.1% positive labels, gradient 1000x stronger along X axis / False Positive Rate. (True Positive / Y axis gradients essentially ignored)

## Gradients using balanced sample weights, proposed loss



- ▶ Left: gradient 4x stronger along X axis for sample weights=1. Balanced sample weights mean equal influence for gradients along both axes, based on the current prediction threshold.
- ▶ Right: proposed method computes gradients based on all ROC points, not just the current prediction threshold.

## Stratified fold assignment, 10-fold CV

```
> folds <- function(by){set.seed(1);
+ data.table(label=rep(0:1,c(100,900)))[
+ , fold := sample(rep(1:10,l=.N)), by
+ ][, table(label, fold)]}
> folds()
      fold
label  1   2   3   4   5   6   7   8   9  10
  0 13 13  4 10 13  7 12  8  9 11
  1 87 87 96 90 87 93 88 92 91 89
> folds("label")
      fold
label  1   2   3   4   5   6   7   8   9  10
  0 10 10 10 10 10 10 10 10 10 10
  1 90 90 90 90 90 90 90 90 90 90
```

With stratification by label, we get the same label counts in each fold.

## ML framework feature comparison

| Language<br>Framework | R<br>mlr3 | how?           | python<br>scikit-learn |
|-----------------------|-----------|----------------|------------------------|
| Learners              | multiple  | benchmark_grid | single                 |
| Parallelization       | yes       | mlr3batchmark  | no                     |
| Subsets(proposed)     | yes       | mlr3resampling | no                     |

- ▶ mlr3 supports parallelization over algorithm, data sets, and train/test splits via mlr3batchmark package (ex: SLURM).
- ▶ scikit-learn cross\_validate computes test error for a single algorithm (no special parallelization support).
- ▶ For an example of how to use stratum, subset, and group in mlr3, see “Arizona trees data” section of [https://cloud.r-project.org/web/packages/mlr3resampling/vignettes/Newer\\_resamplers.html](https://cloud.r-project.org/web/packages/mlr3resampling/vignettes/Newer_resamplers.html)
- ▶ Scikit-learn [https://scikit-learn.org/stable/modules/cross\\_validation.html#stratifiedgroupkfold](https://scikit-learn.org/stable/modules/cross_validation.html#stratifiedgroupkfold) supports group, and stratification by class, but not subset.