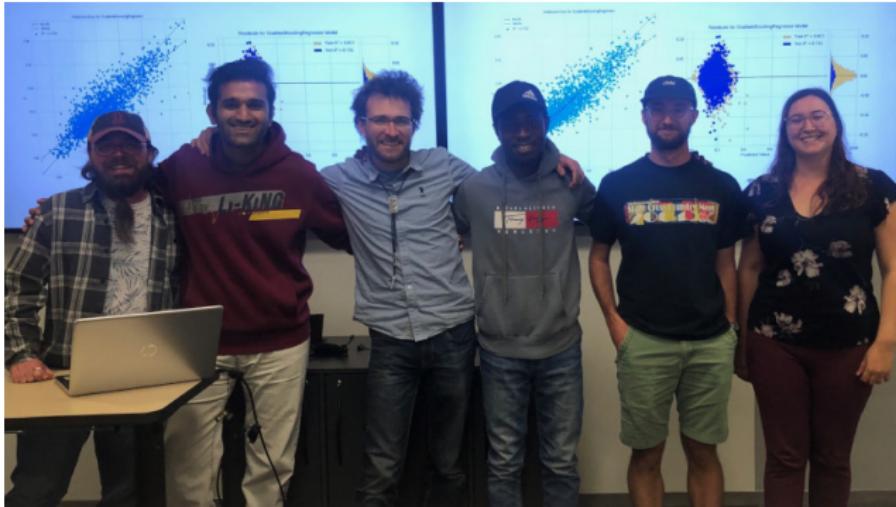


Two new algorithms for scientific applications of machine learning

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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 Train Learned Predictions
Algorithm data function on test data

Learn() $\rightarrow g$ $g(\text{ } \square) = 0$
 $g(\text{ } \blacksquare) = 1$
 $g(\text{ } \blacksquare \blacksquare) = 1$

Learn() $\rightarrow h$ $h(\text{ } \blacksquare) = 0$
 $h(\text{ } \blacksquare \blacksquare) = 0$
 $h(\text{ } \blacksquare \blacksquare \blacksquare) = 1$

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



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

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?

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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)

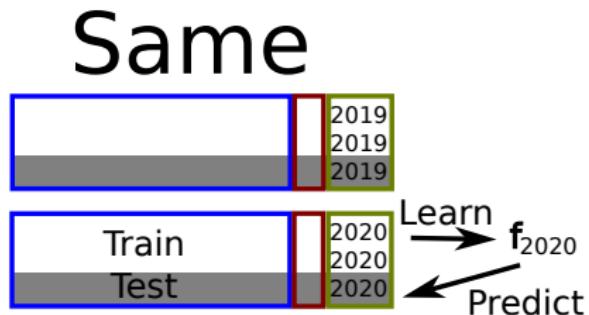
- ▶ Example: childhood autism prediction data set.
- ▶ Subsets of interest are years, which can be represented by adding a new column to the data table.

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 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 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

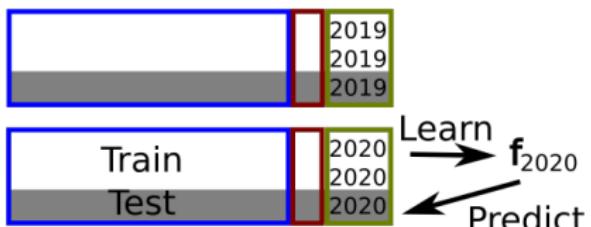
- Compare Same and Other error when predicting on test subset (2020)
- If subsets are similar, (2019 data are useful for learning how to predict in 2020) then the larger subset (Same or Other) should have smaller test error

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.

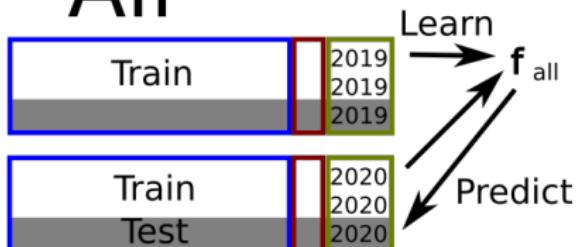
People	Inputs Questions	D	Autism	Year
			1	N
1			0	2019
			0	2019
			1	2019
			0	2020
			1	2020
			1	2020

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



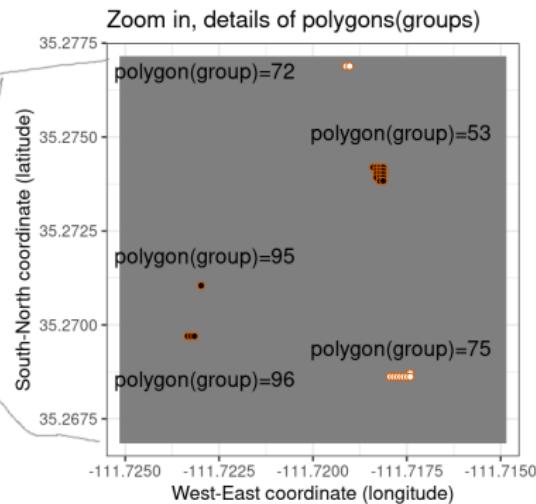
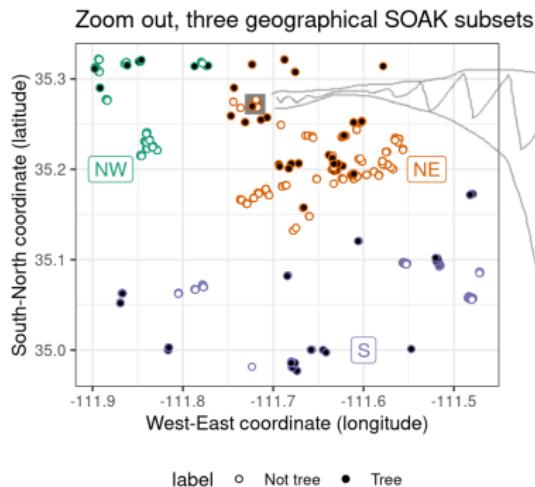
Proposed SOAK algorithm (generic data)

- ▶ 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).

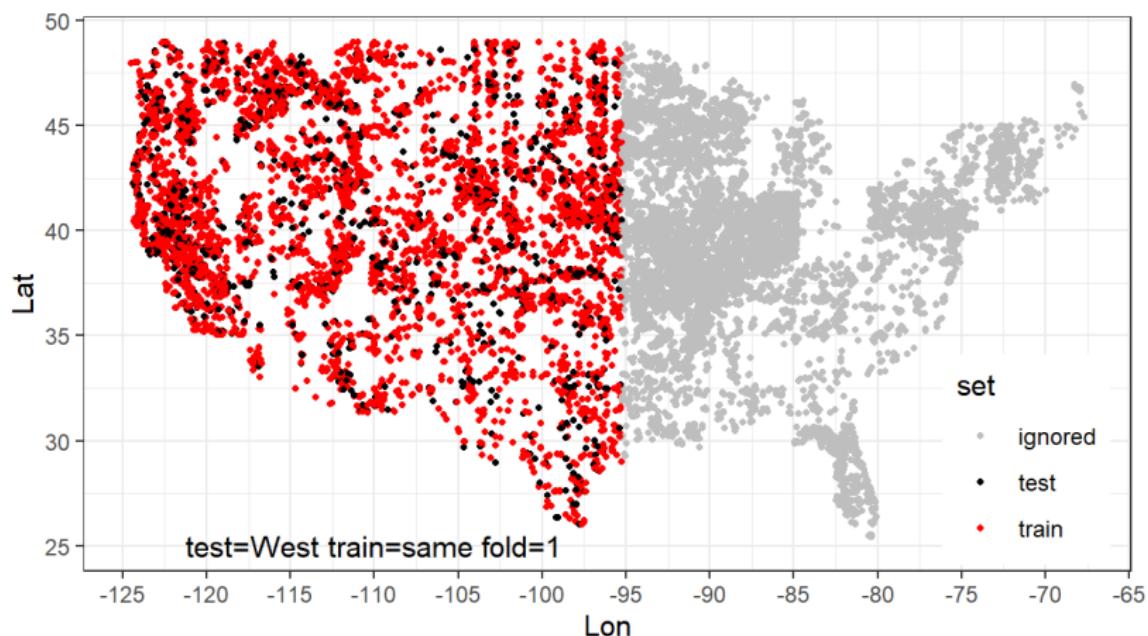


Proposed SOAK algorithm new to ML frameworks

- ▶ 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)

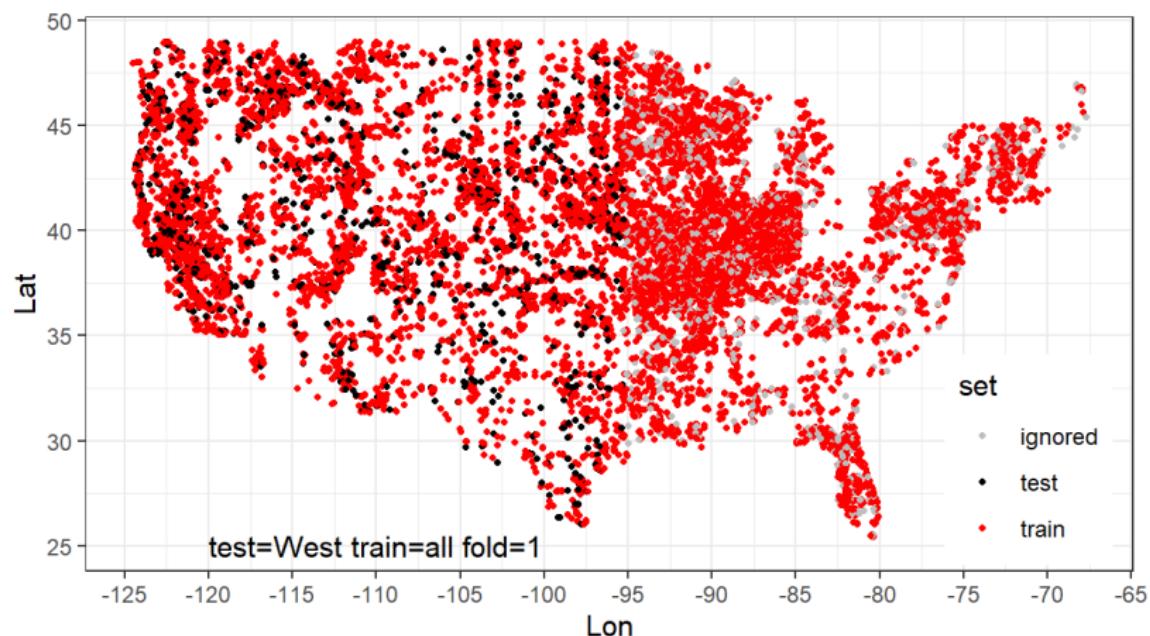


Proposed SOAK algorithm (geographical data example)



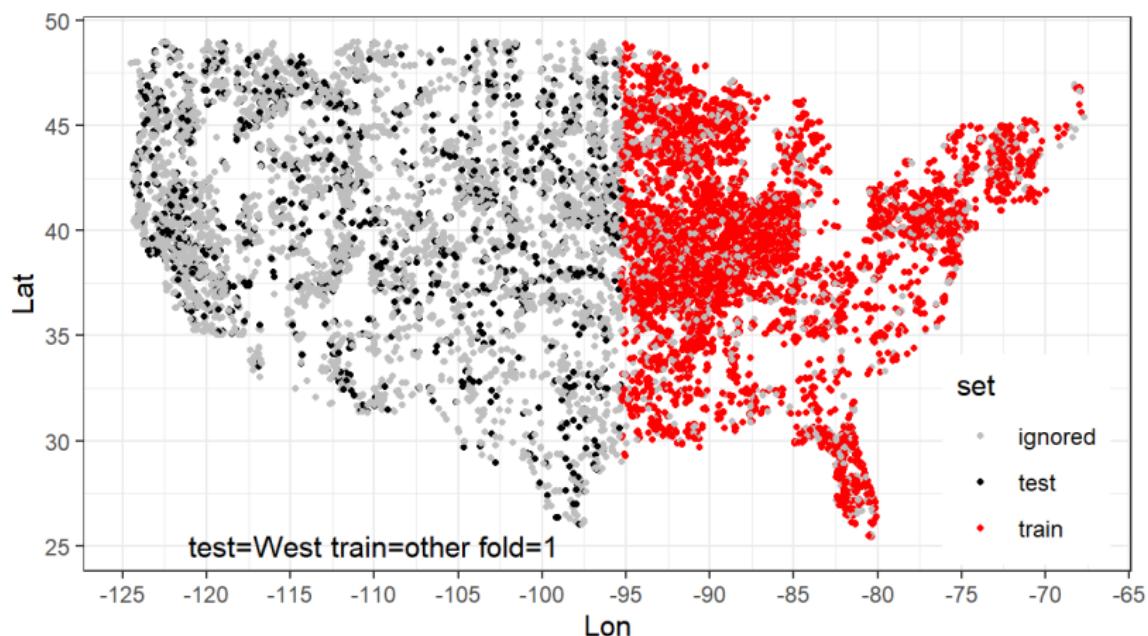
- ▶ Say we want good prediction in western USA.
- ▶ One of the K test sets is: subset=West and fold=1.
- ▶ Train on Same (West, fold \neq 1) establishes a baseline.

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)

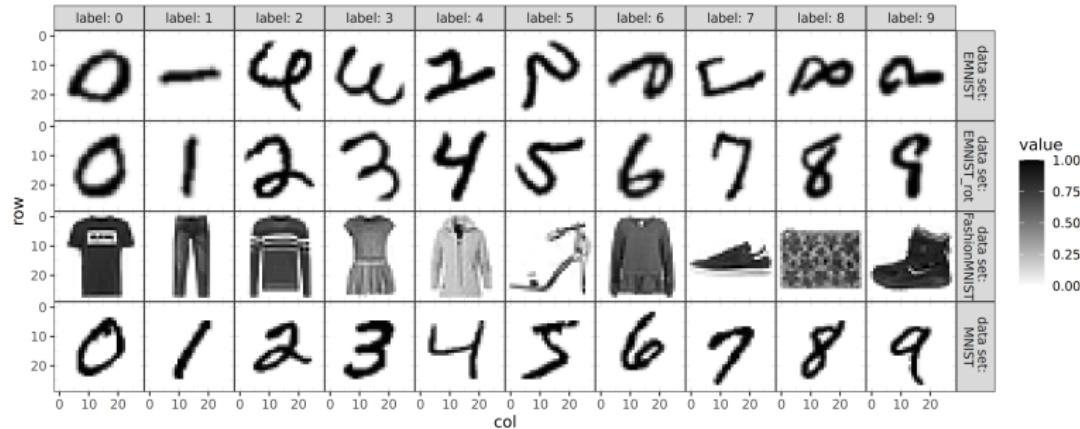


- ▶ Train on Other (East, $\text{fold} \neq 1$) would be less accurate than Same if subsets are different.
- ▶ If subsets are similar, then the larger of Same and Other should be more accurate (more relevant training data).

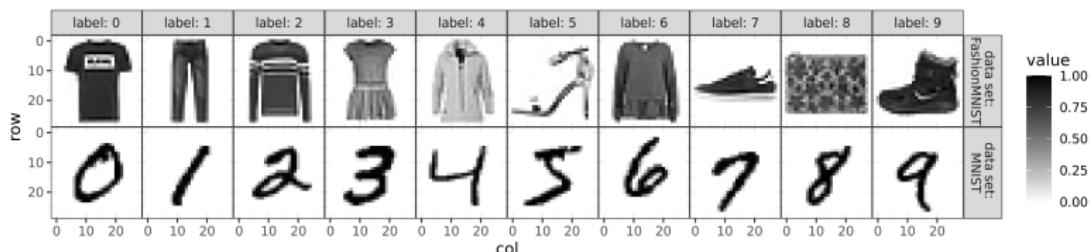
ImagePair data: train on MNIST and accurately predict on MNIST variants?



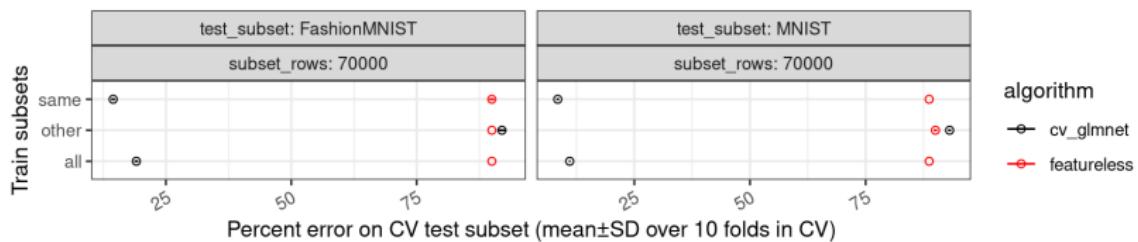
- ▶ Expect: $g(\text{boot})$ and $h(\text{circle})$ are not accurate.
- ▶ But train on MNIST, predict on EMNIST_rot (upright digits) should be possible, right? (Vote!) Let's use SOAK to find out!
- ▶ Create three new IPair data sets by combining MNIST with variants: EMNIST, EMNIST_rot, FashionMNIST.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



SOAK for MNIST+FashionMNIST (IPair_Fashion data set)

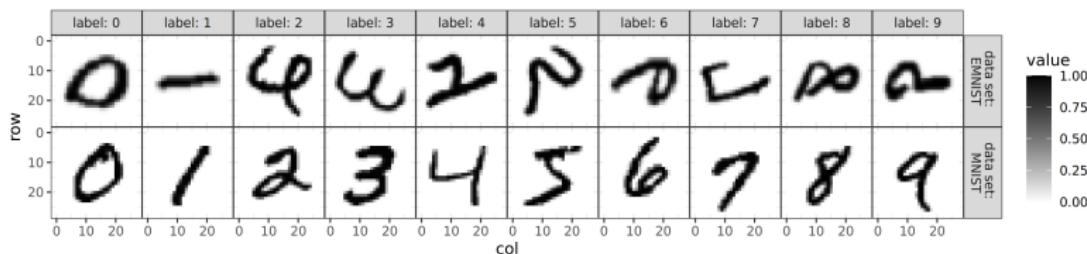


Data set: MNIST_FashionMNIST

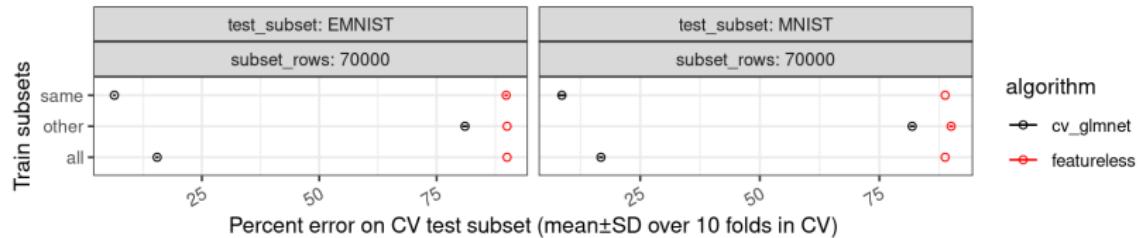


- ▶ **cv_glmnet** is L1-regularized linear model.
- ▶ **featureless** baseline always predicts most frequent class.
- ▶ Other **cv_glmnet** has greater test error than **featureless**.
- ▶ The patterns in the two subsets are too different for **Other cv_glmnet** to learn anything useful for prediction.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

SOAK for MNIST+EMNIST (IPair_E data set)

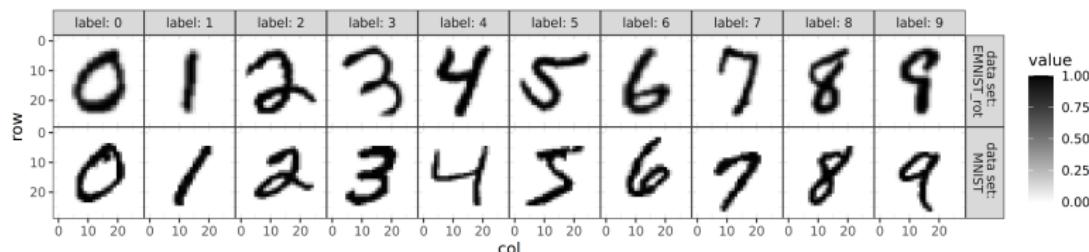


Data set: MNIST_EMNIST

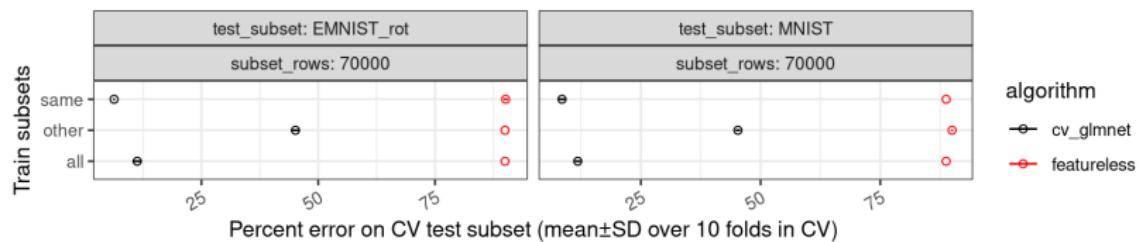


- ▶ **Other cv_glmnet** has significantly smaller test error than **featureless**, so linear model learns something that useful for predicting on the other subset.
- ▶ But since **Other** error rate is much larger than **Same**, clearly the pattern is very different between MNIST/EMNIST.

SOAK for MNIST+EMNIST_rot (IPair_E_rot data set)



Data set: MNIST_EMNIST_rot

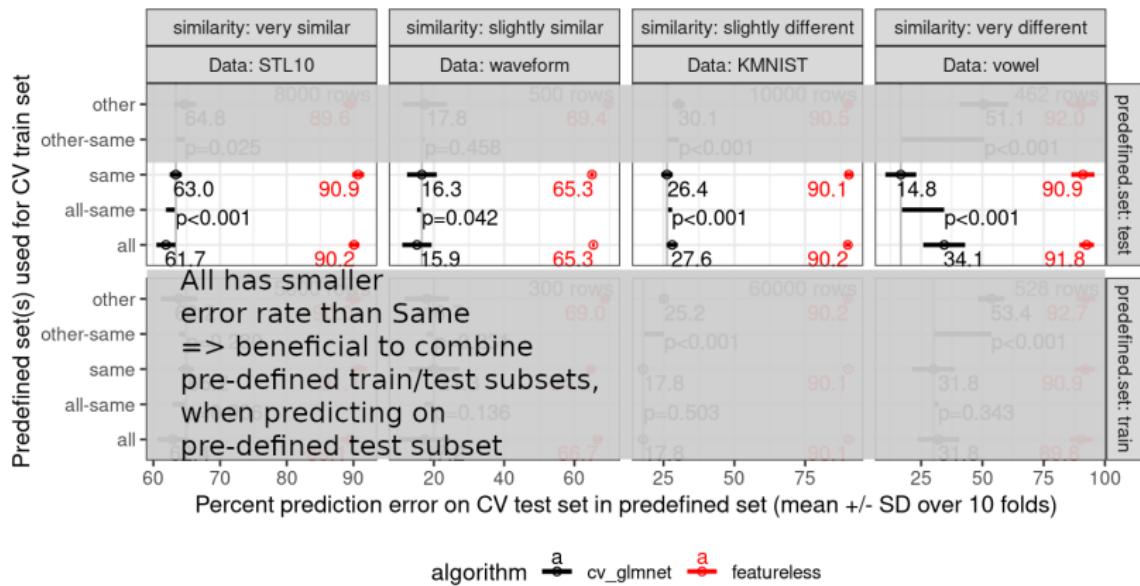


- ▶ Other cv_glmnet has even smaller test error, indicating even more similarity between MNIST and EMNIST_rot data sets.
- ▶ But Other/All test error are still not as small as Same.
- ▶ Significant difference between patterns learnable/predictable by linear model in MNIST/EMNIST_rot. (surprising)

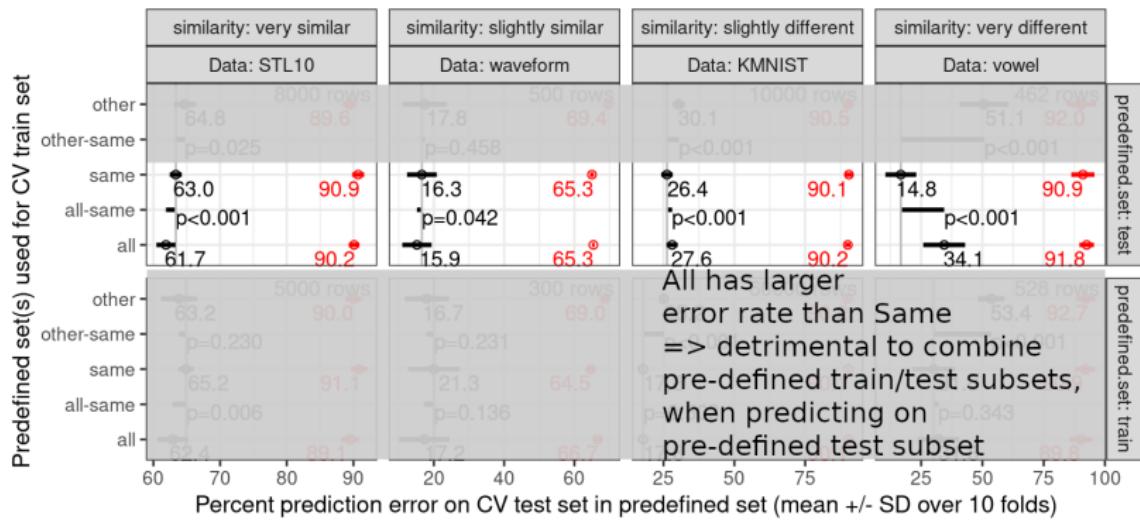
Benchmark data with pre-defined train/test subsets

- ▶ 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

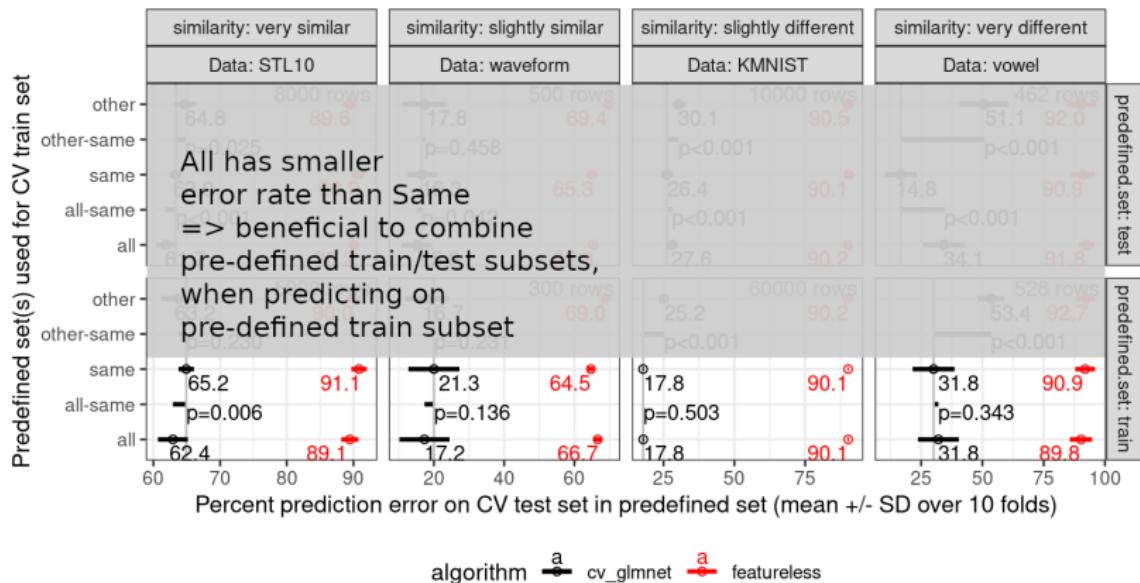


Benchmark data with pre-defined train/test subsets

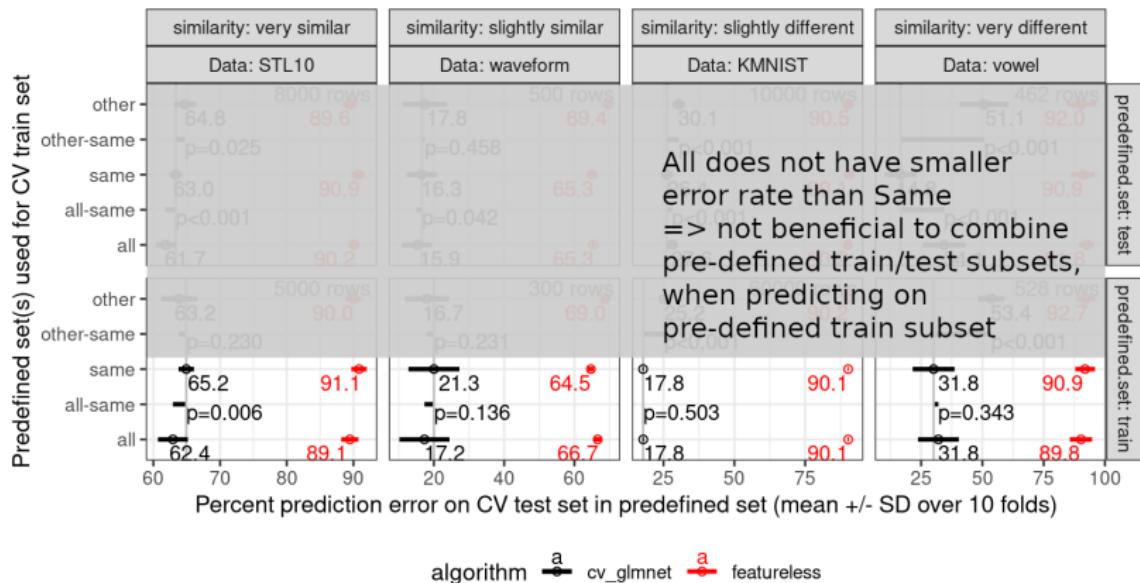


algorithm cv_glmnet featureless

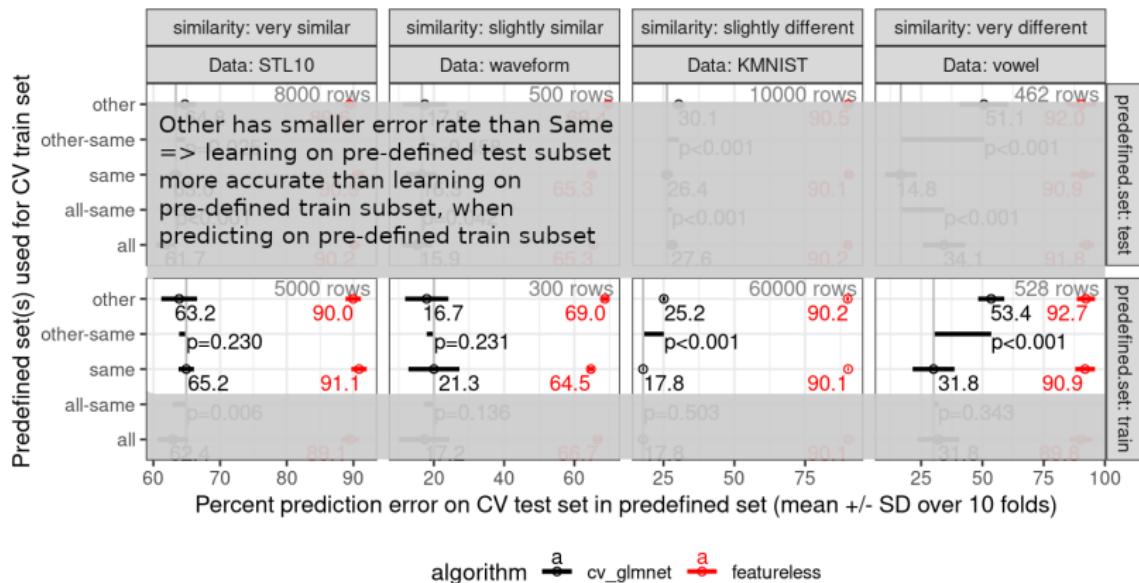
Benchmark data with pre-defined train/test subsets



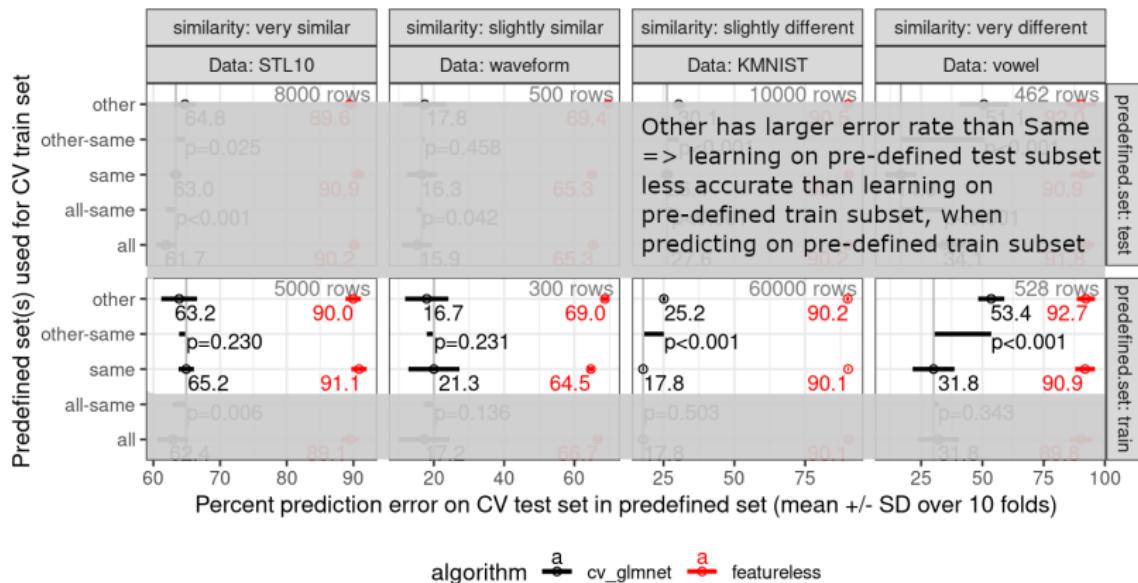
Benchmark data with pre-defined train/test subsets



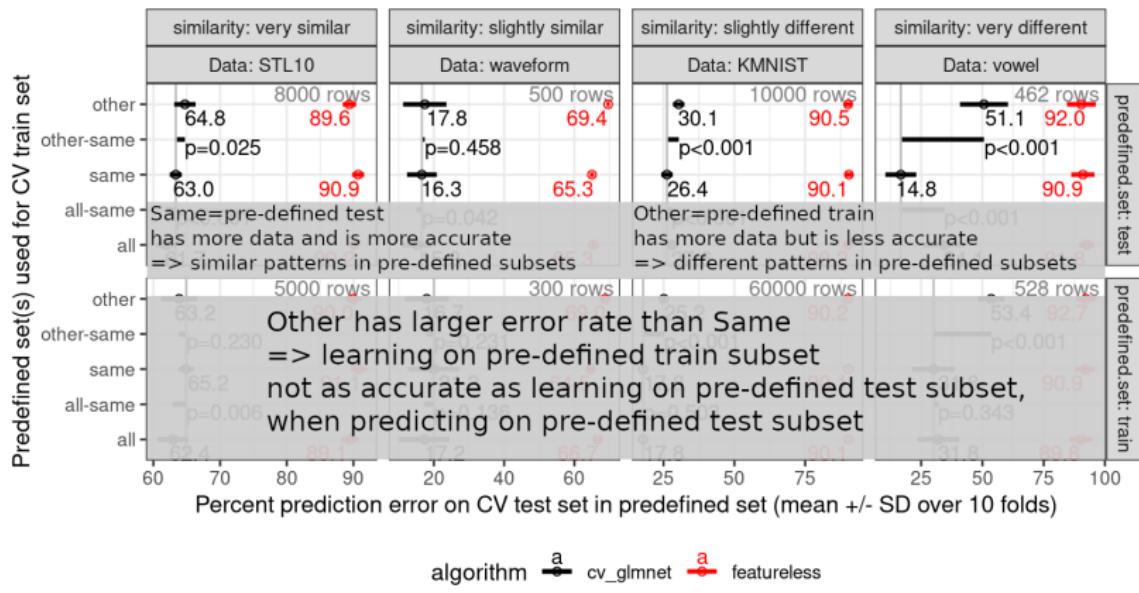
Benchmark data with pre-defined train/test subsets



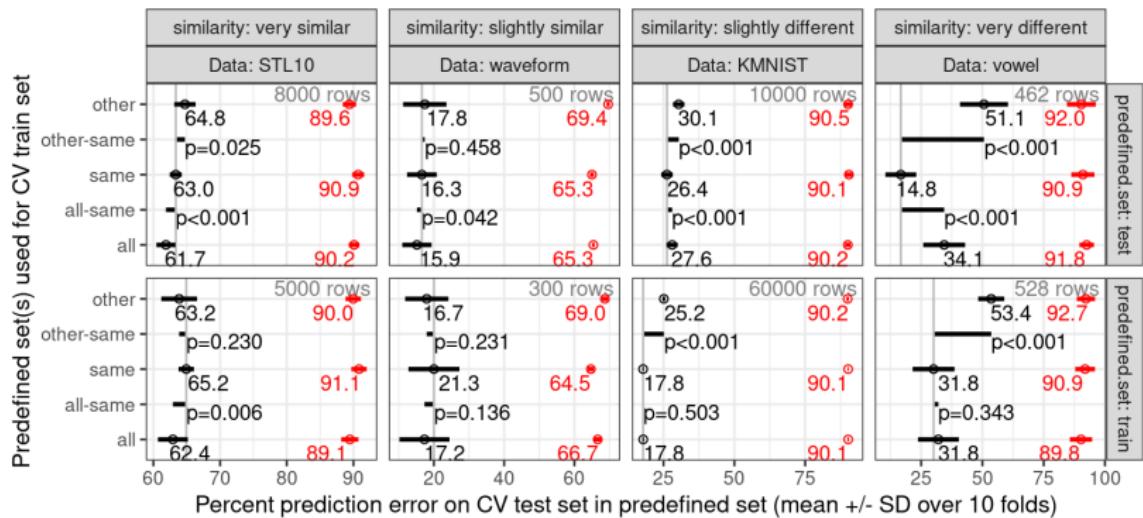
Benchmark data with pre-defined train/test subsets



Benchmark data with pre-defined train/test subsets



Benchmark data with pre-defined train/test subsets



algorithm cv_glmnet featureless

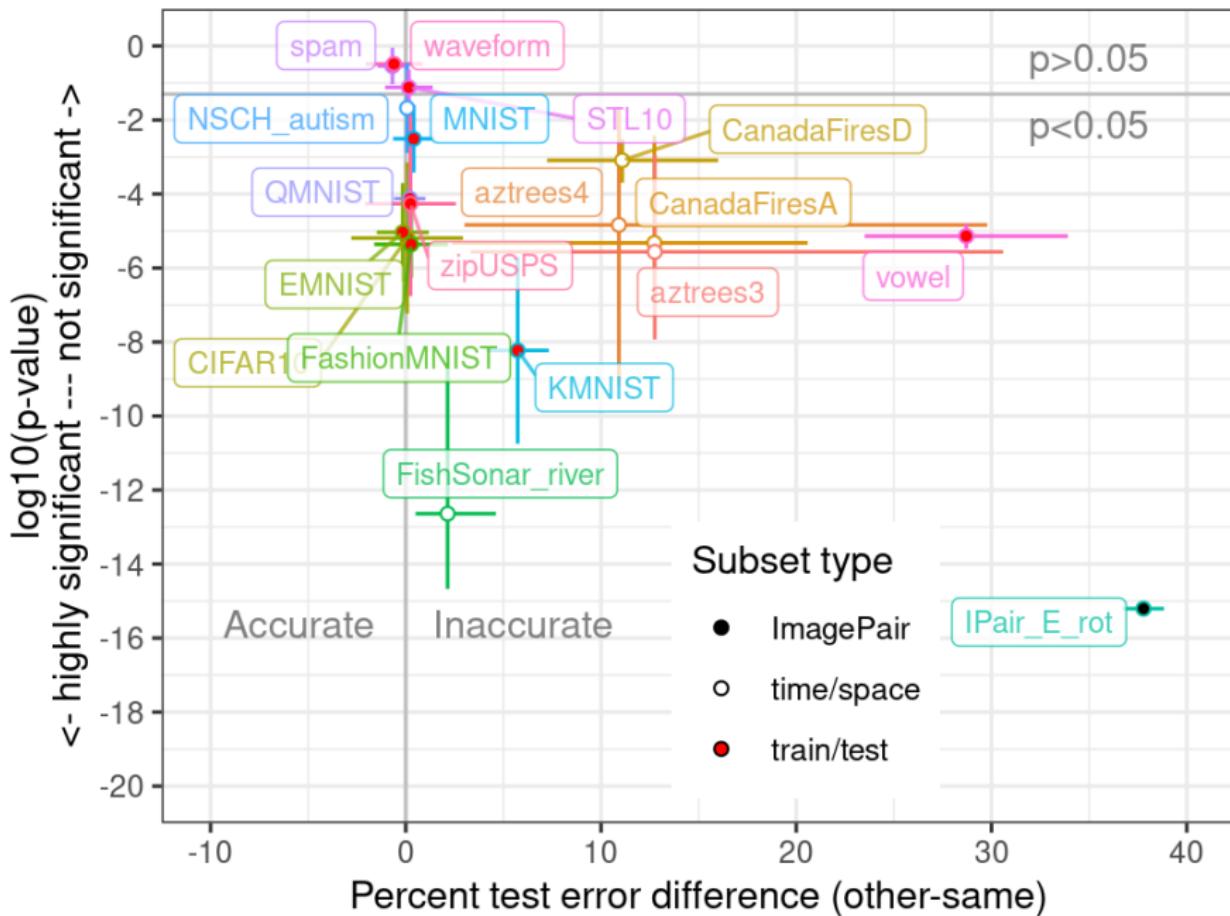
- ▶ Left data sets have similar pre-defined train/test subsets (expected), All error is always less than Same, and Other error is either greater or less than Same, depending on subset sizes.
- ▶ Right data sets have different pre-defined train/test subsets (surprising), All error is always greater than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

20 classification data sets analyzed using SOAK

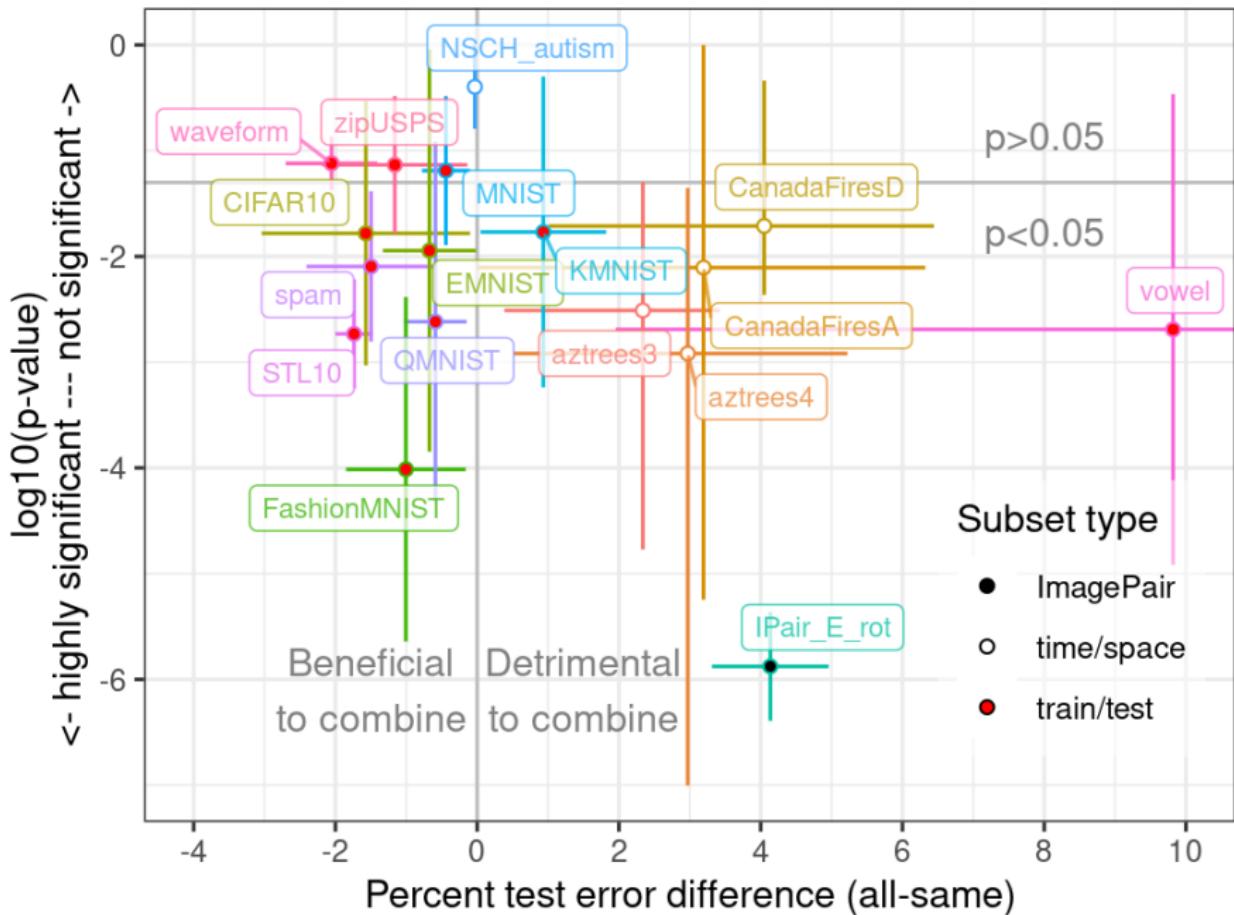
We considered MNIST and variants as subsets (**ImagePair**),
data from collaborations (**time/space** subsets),
and benchmark data with pre-defined **train/test** subsets.

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?



Discussion and Conclusions

- ▶ 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**).
- ▶ 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.
- ▶ Most pre-defined train/test subsets in benchmark data are

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Train on one subset and accurately predict on another?

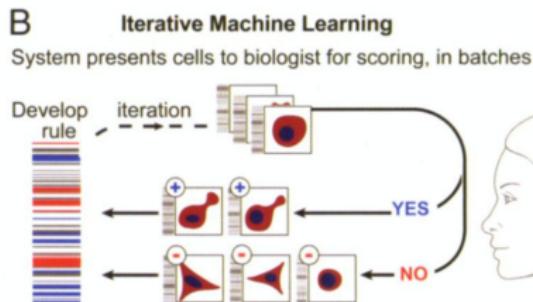
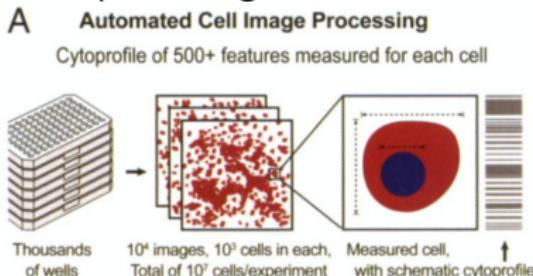
SOAK: Same/Other/All K-fold cross-validation for estimating similarity of patterns in data subsets (arXiv:2410.08643)

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.

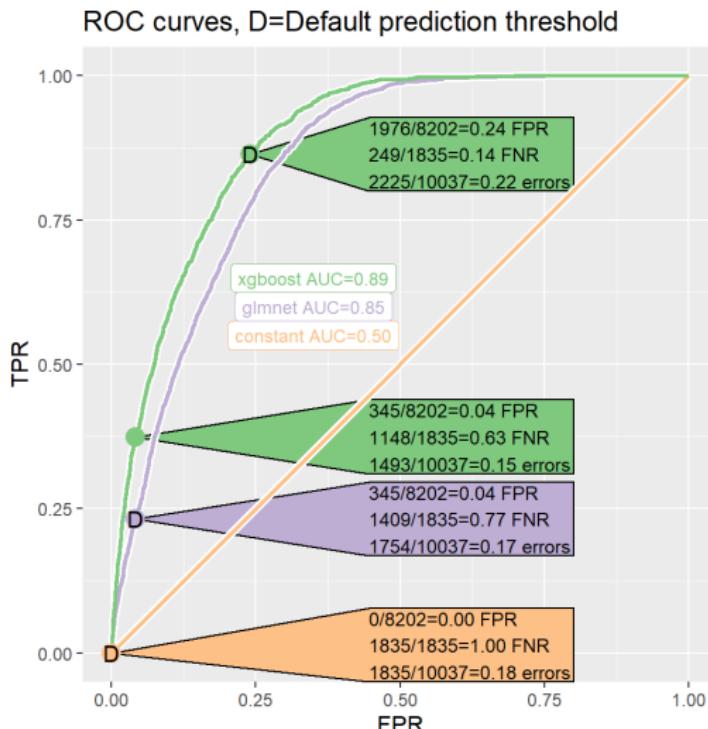


Gradient descent algorithms (Logistic regression, SVM, etc) minimize a differentiable surrogate of zero-one loss = sum of:

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).

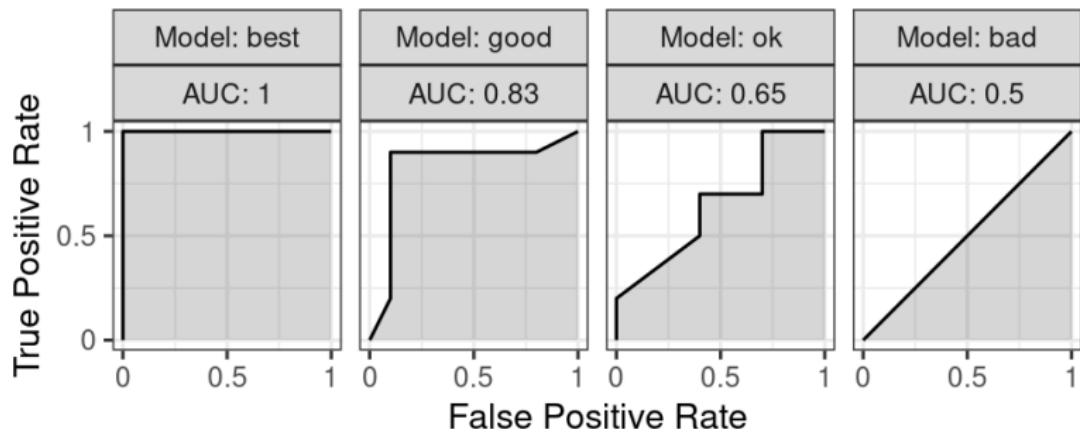
ROC curves: fair comparison with different default FPR



- ▶ 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

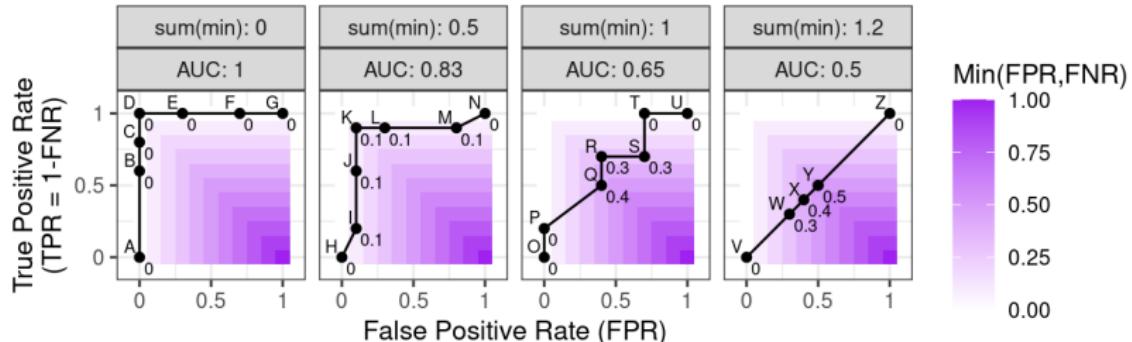
- ▶ Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- ▶ ROC curve of learned f is plot of True Positive Rate vs False Positive Rate: each point on the ROC curve is a different constant $c \in \mathbb{R}$ added to the predicted values: $f(\mathbf{x}) + c$.
- ▶ $c = \infty$ 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

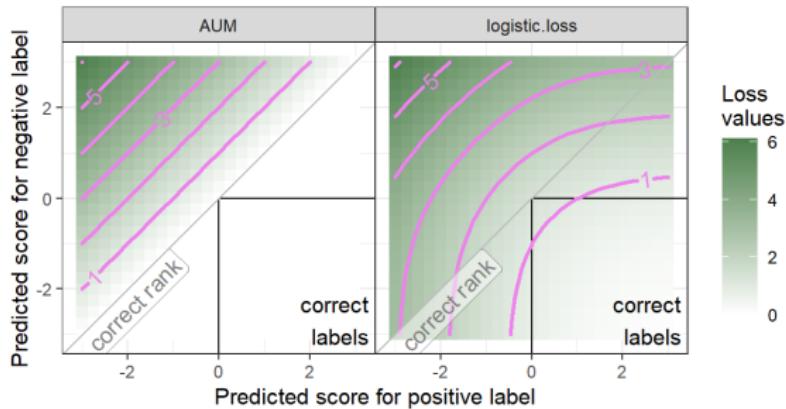
Can we learn a binary classification function f which directly optimizes the ROC curve?

- ▶ 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 $\min(\text{FPR}, \text{FNR})$.

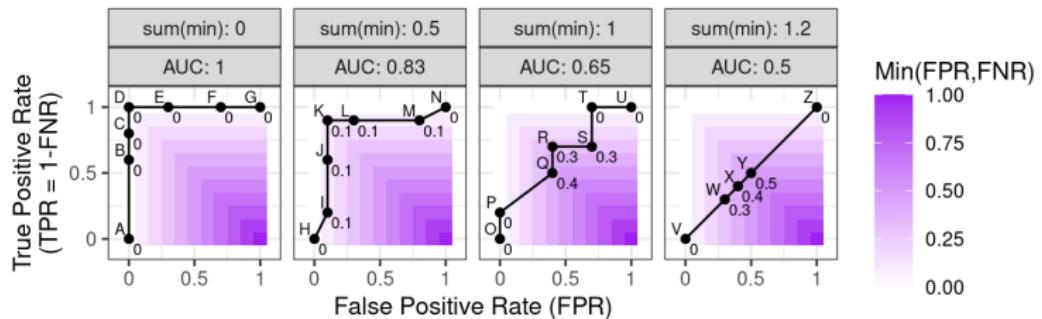


Comparing proposed loss with baselines

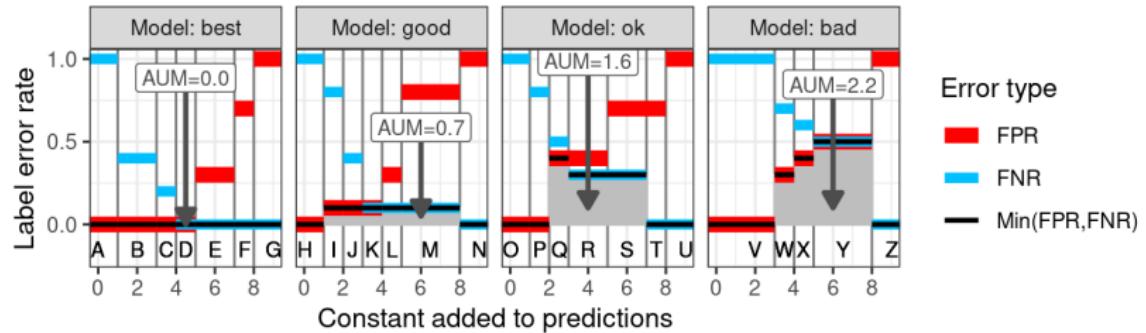
- ▶ Classic baselines: hinge and logistic loss, sum over samples, $\ell[yf(x)]$.
- ▶ Bamber (1975) proved ROC-AUC relation to Mann-Whitney U statistic (double sum over all pairs of positive and negative samples).
- ▶ Recently: SVM^{struct} (Joachims 2005), X-risk (Yang 2022), All Pairs Squared Hinge (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)

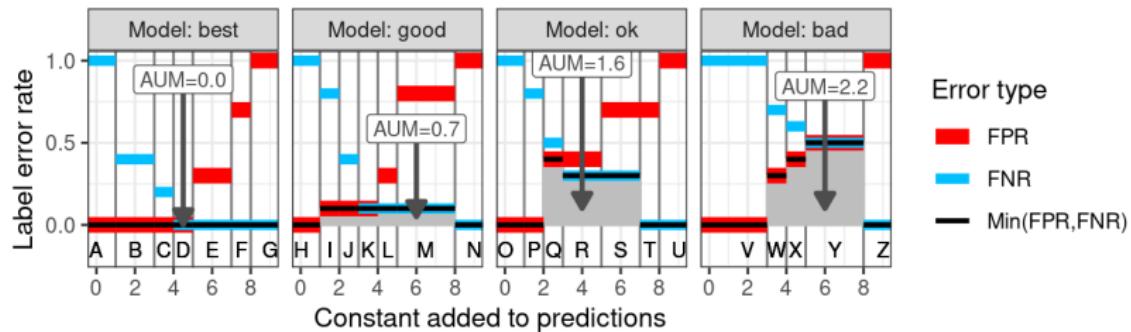


Above: purple heat map = numbers near dots = distance to top or left
= same as black min error rate functions below.



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

Computing Sum of Min (SM) over all ROC points

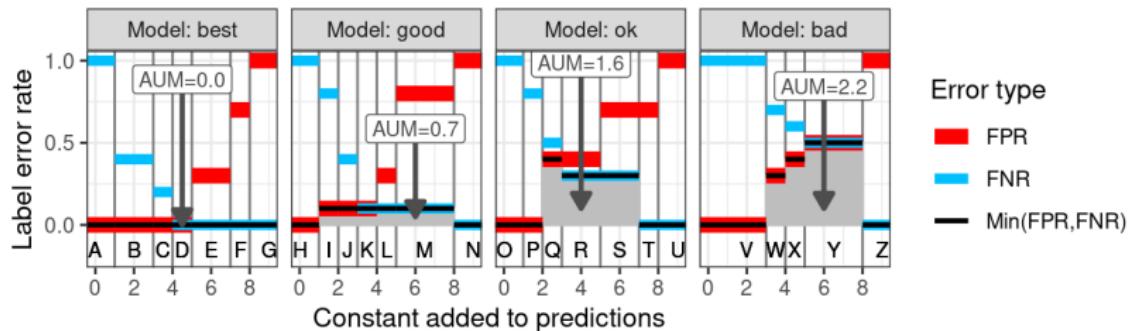


- ▶ For N samples, there are $\leq N + 1$ points on the ROC curve,
- ▶ with sorted thresholds of c , $T_1 \leq \dots \leq T_N \in \mathbb{R}$ (grey lines),
- ▶ and corresponding min error values M_2, \dots, M_N (black).
- ▶ Then if I is the indicator function, we can write the sum of the min (SM), over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

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

(\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

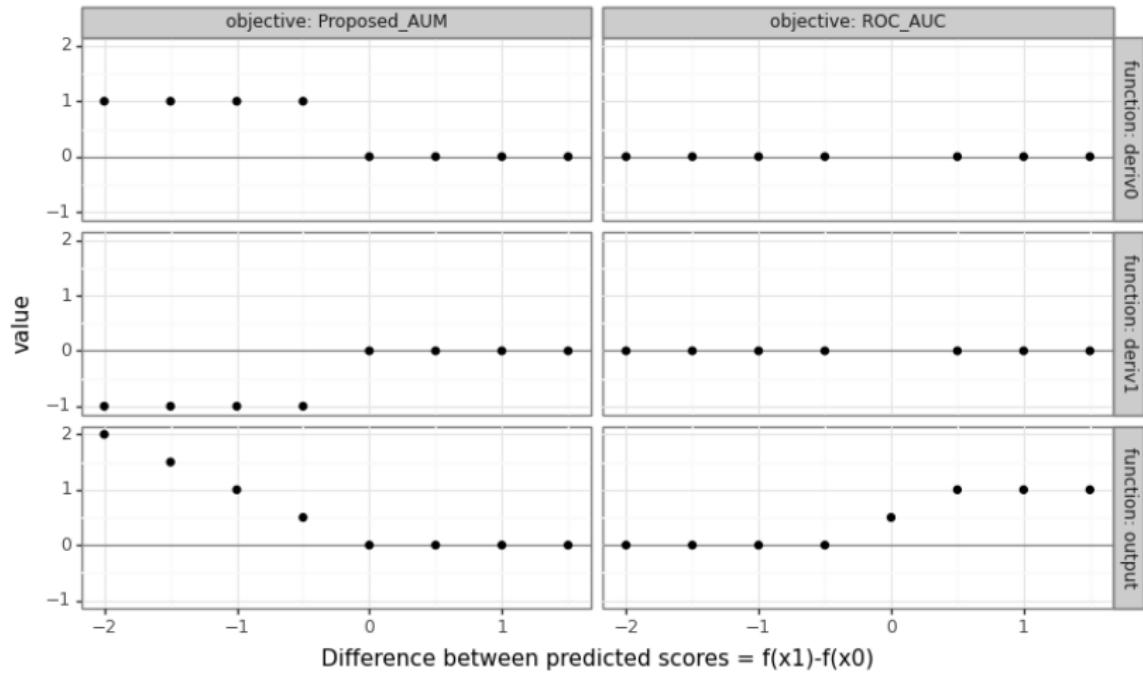
```
def ROC_AUC(pred_tensor, label_tensor):
    "Classic metric, but gradient zero almost everywhere"
    roc = ROC_curve(pred_tensor, label_tensor)
    FPR_diff = roc["FPR"] [1:]-roc["FPR"] [: -1]
    TPR_sum = roc["TPR"] [1:]+roc["TPR"] [: -1]
    return torch.sum(FPR_diff*TPR_sum/2.0)

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)
```

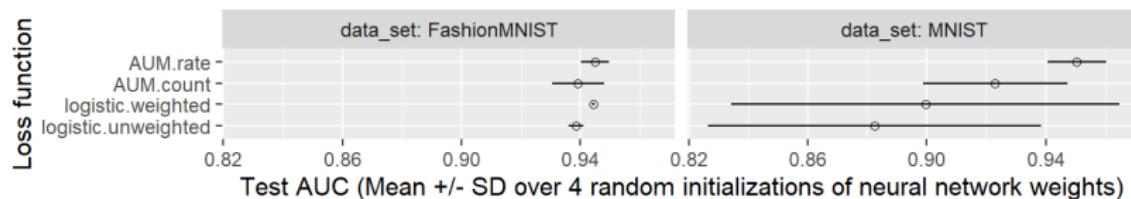
<https://tdhock.github.io/blog/2024/torch-roc-aum/>

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.

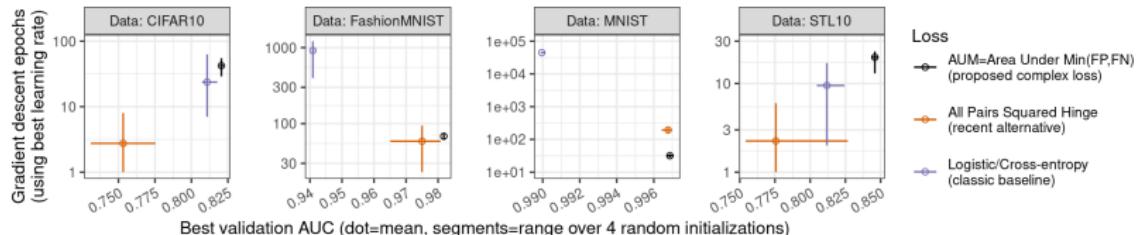


Comparing proposed AUM with weighted logistic loss



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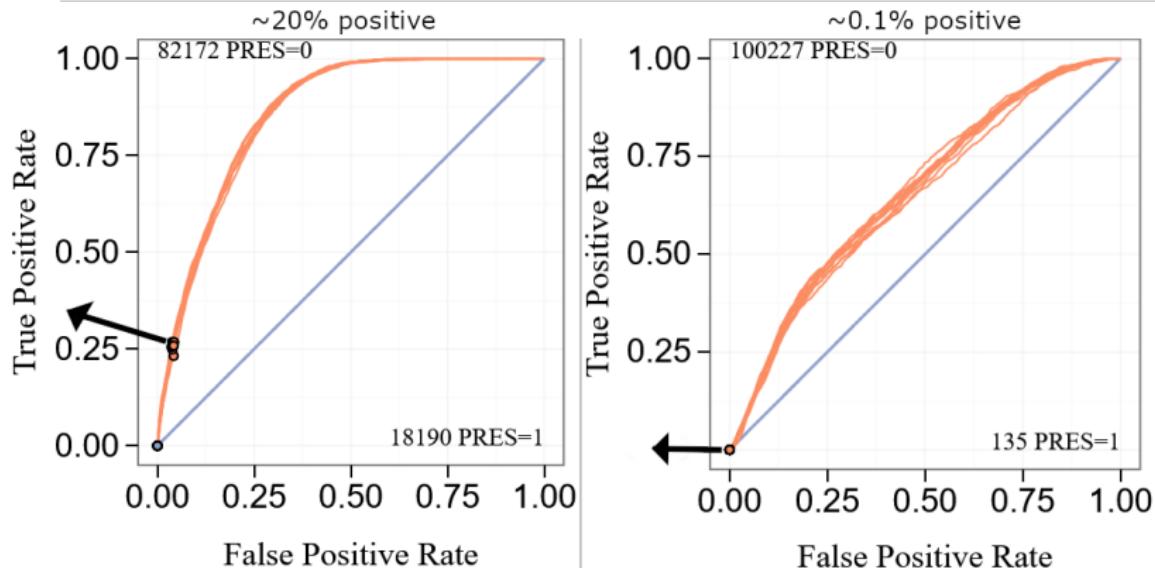


Reproducible slide/figure source code:

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

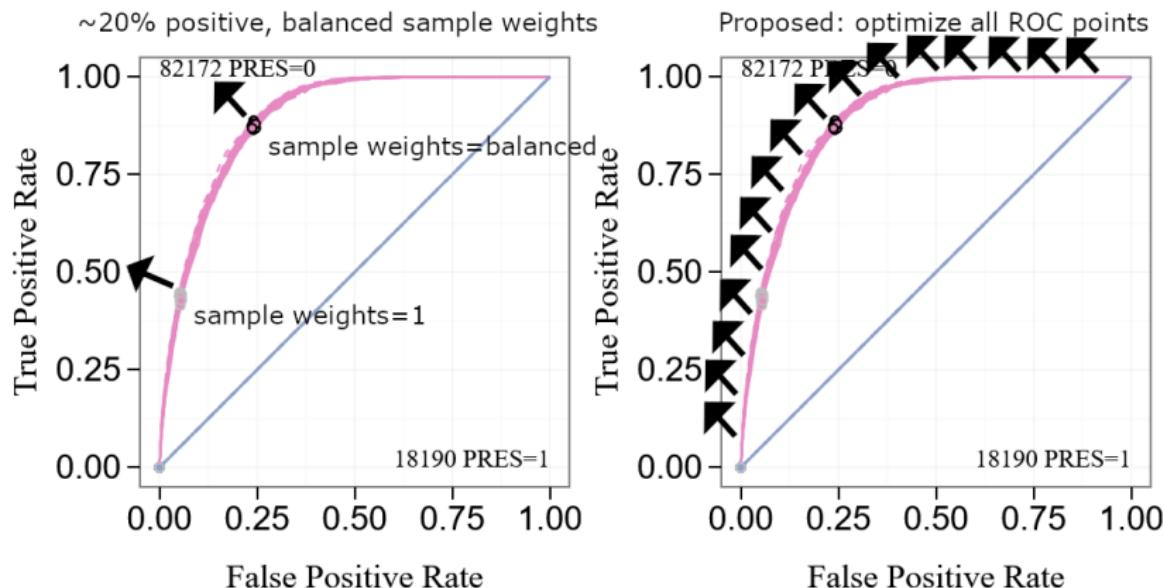
<https://github.com/tdhock/max-generalized-auc>

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.