Two new algorithms for scientific applications of machine learning

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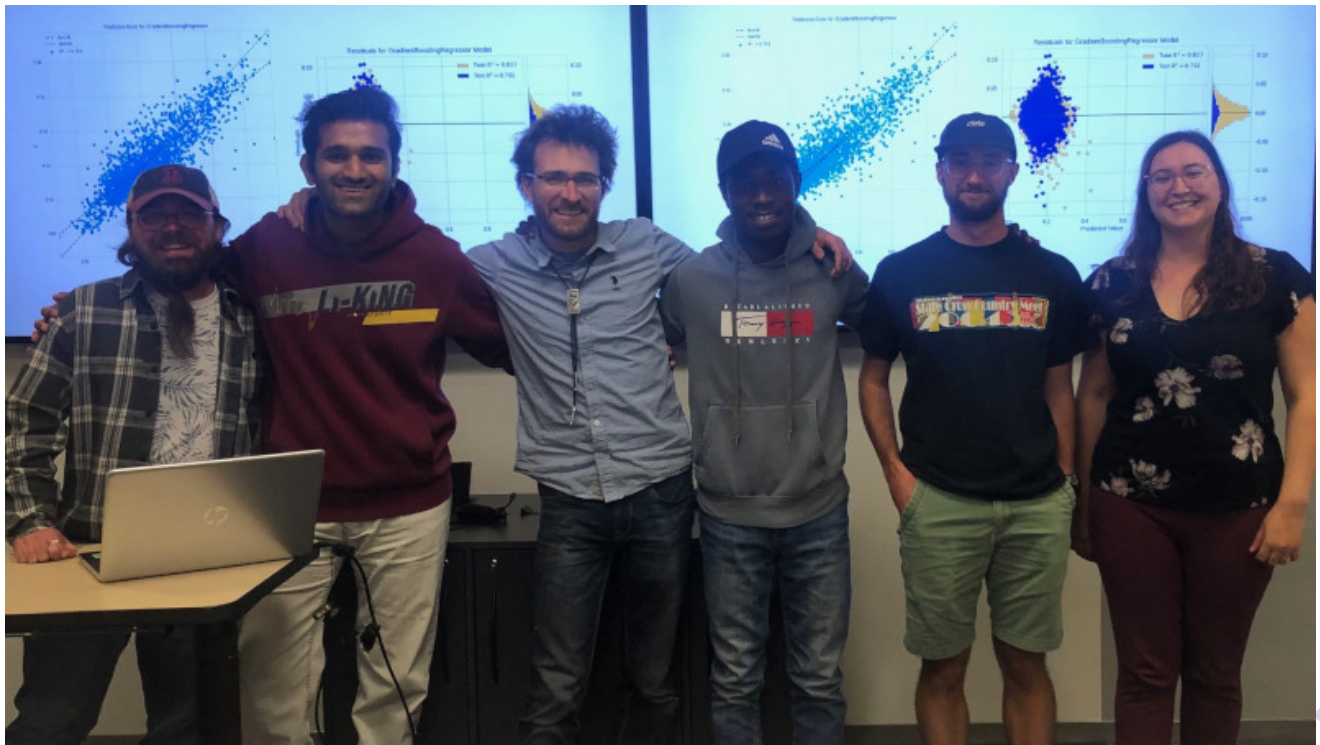


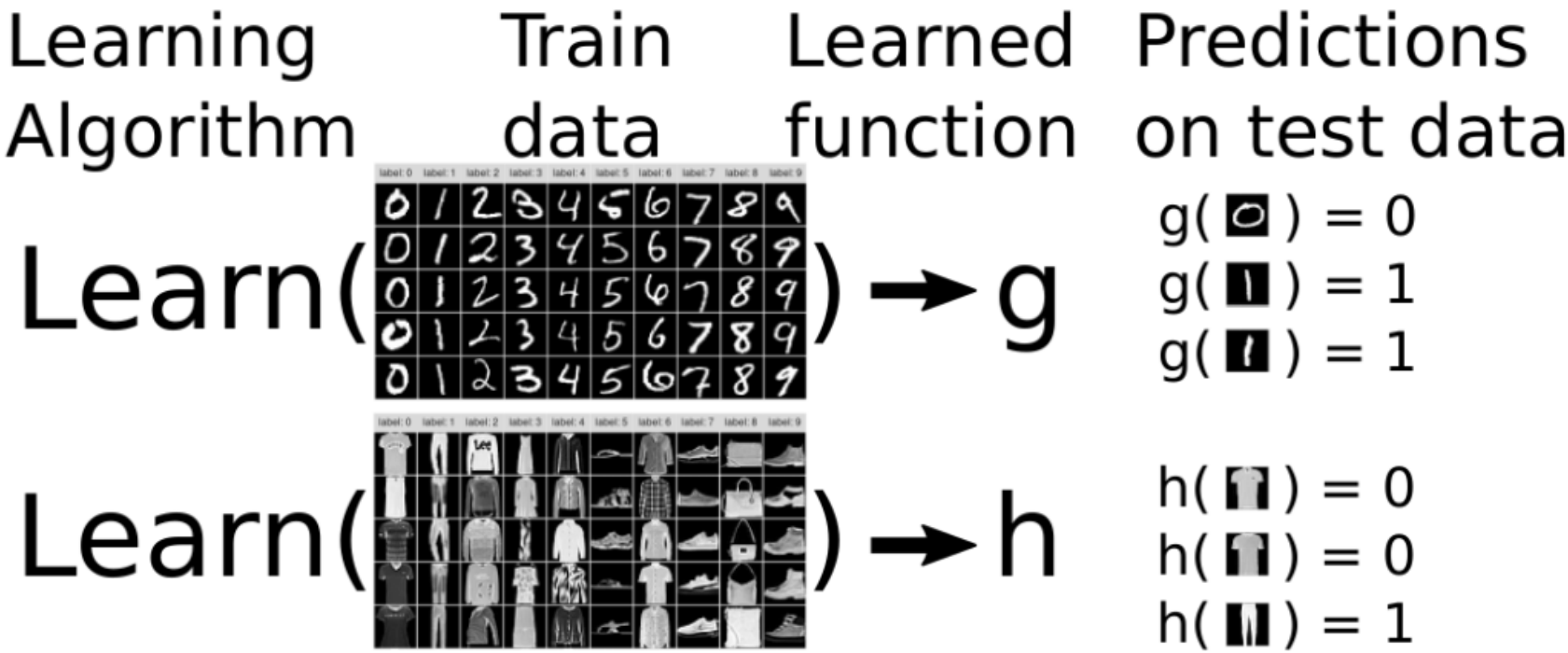
Introduction: two common questions in collaborations involving applications of machine learning

SOAK: Same/Other/All K-fold cross-validation for comparing models trained on data subsets

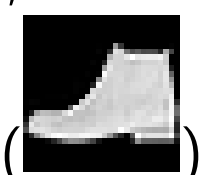
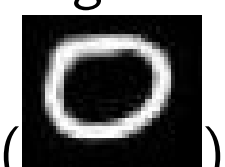
AUM=Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization

Learning two different functions using two data sets

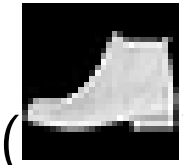
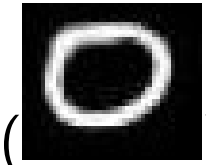
Figure from chapter by Hocking TD, *Introduction to machine learning and neural networks* for book *Land Carbon Cycle Modeling: Matrix Approach, Data Assimilation, and Ecological Forecasting* edited by Luo Y (Taylor and Francis, 2022).



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

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

Train on one subset and accurately predict on another?

- What if you do $g($  $)$, or $h($  $)$?
- This is a question about **generalization**: how accurate is the learned function on a new/test data set?
- "Very accurate" if test data are similar enough to train data (best case is i.i.d. = independent and identically distributed)
- Predicting childhood autism (Lindly *et al.*), train on one year of surveys, test on another.
- Predicting carbon emissions (Aslam *et al.*), train on one city, test on another.
- Predicting presence of trees/burn 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 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?

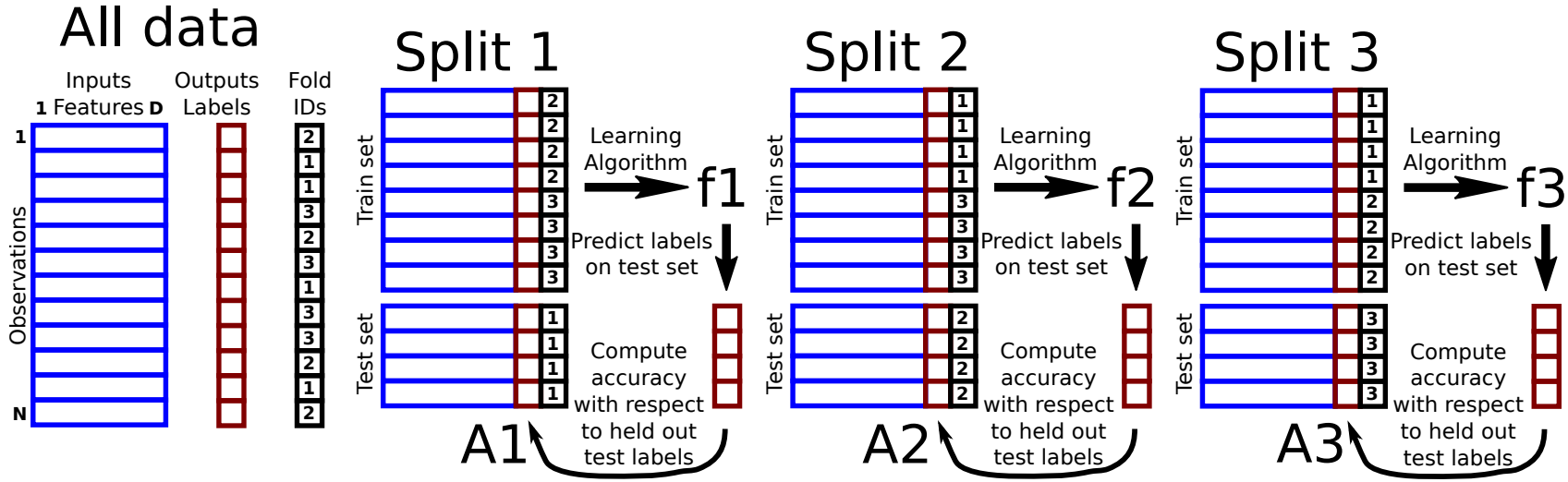
Introduction: two common questions in collaborations involving applications of machine learning

SOAK: Same/Other/All K-fold cross-validation for comparing models trained on data subsets

AUM=Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization

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.



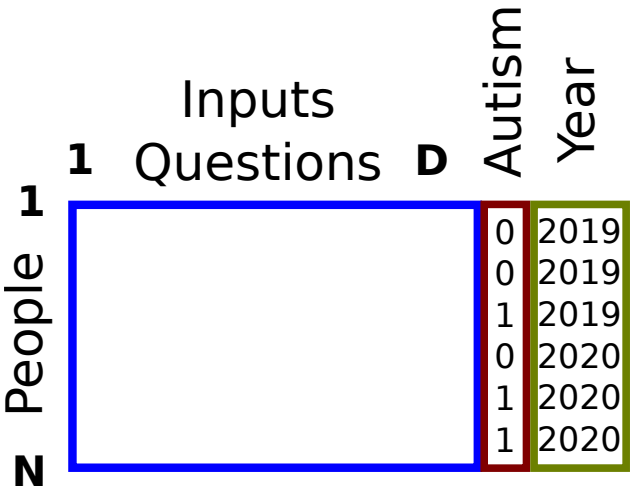
Hocking TD *Intro. to machine learning and neural networks* (2022).

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

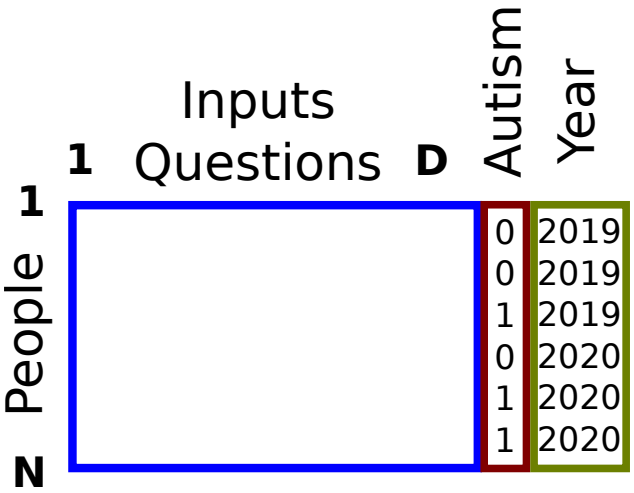
Proposed SOAK algorithm (Autism data example)

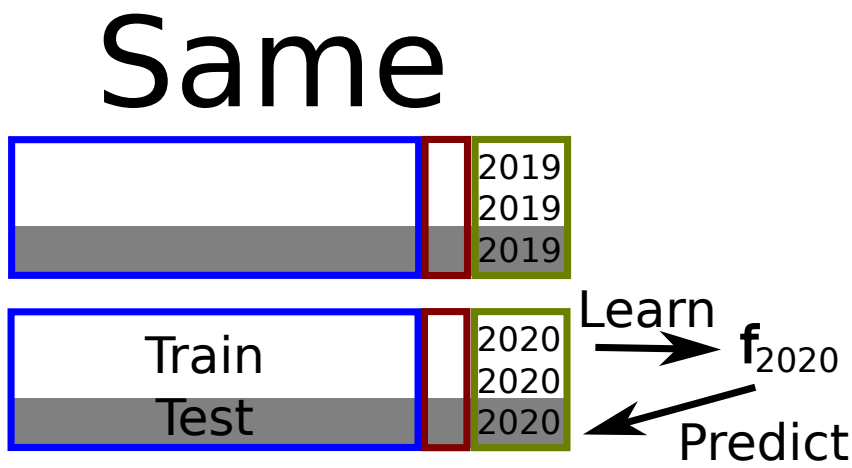
- Example: childhood autism prediction data set.



Proposed Same Other Cross-Validation

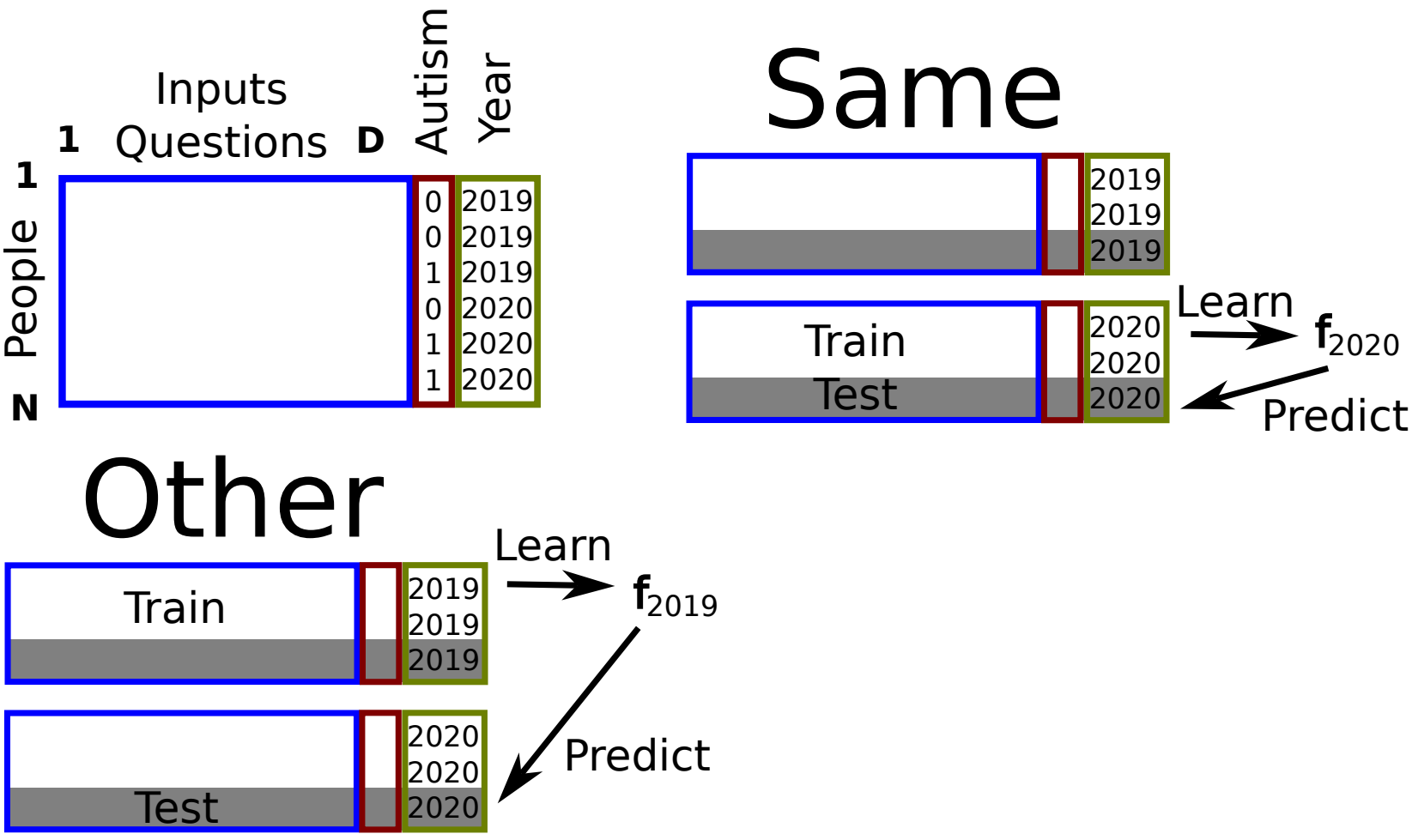
- Train subset same as test (=regular K-fold CV on 2020).





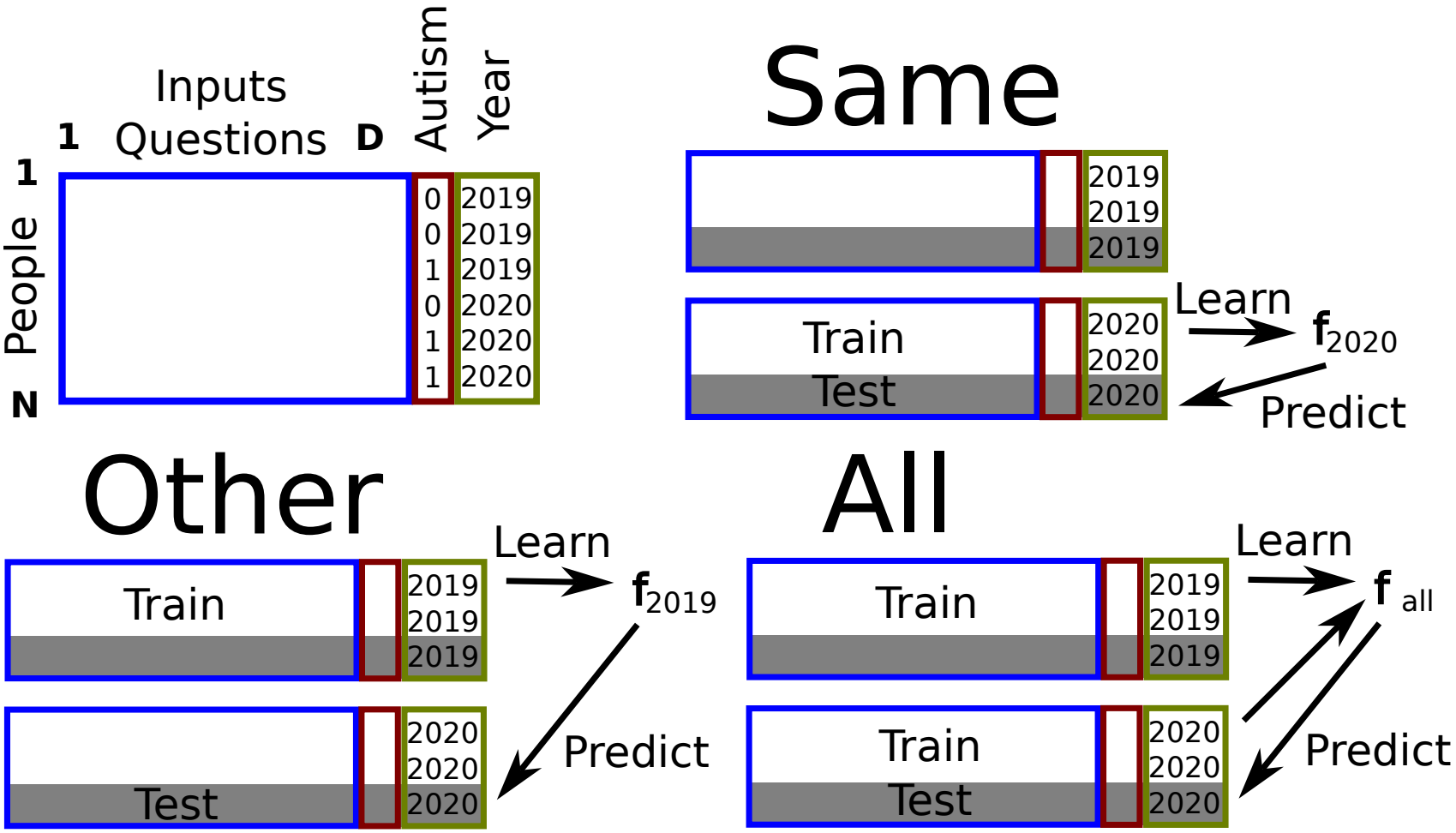
Proposed SOAK algorithm (Autism data example)

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



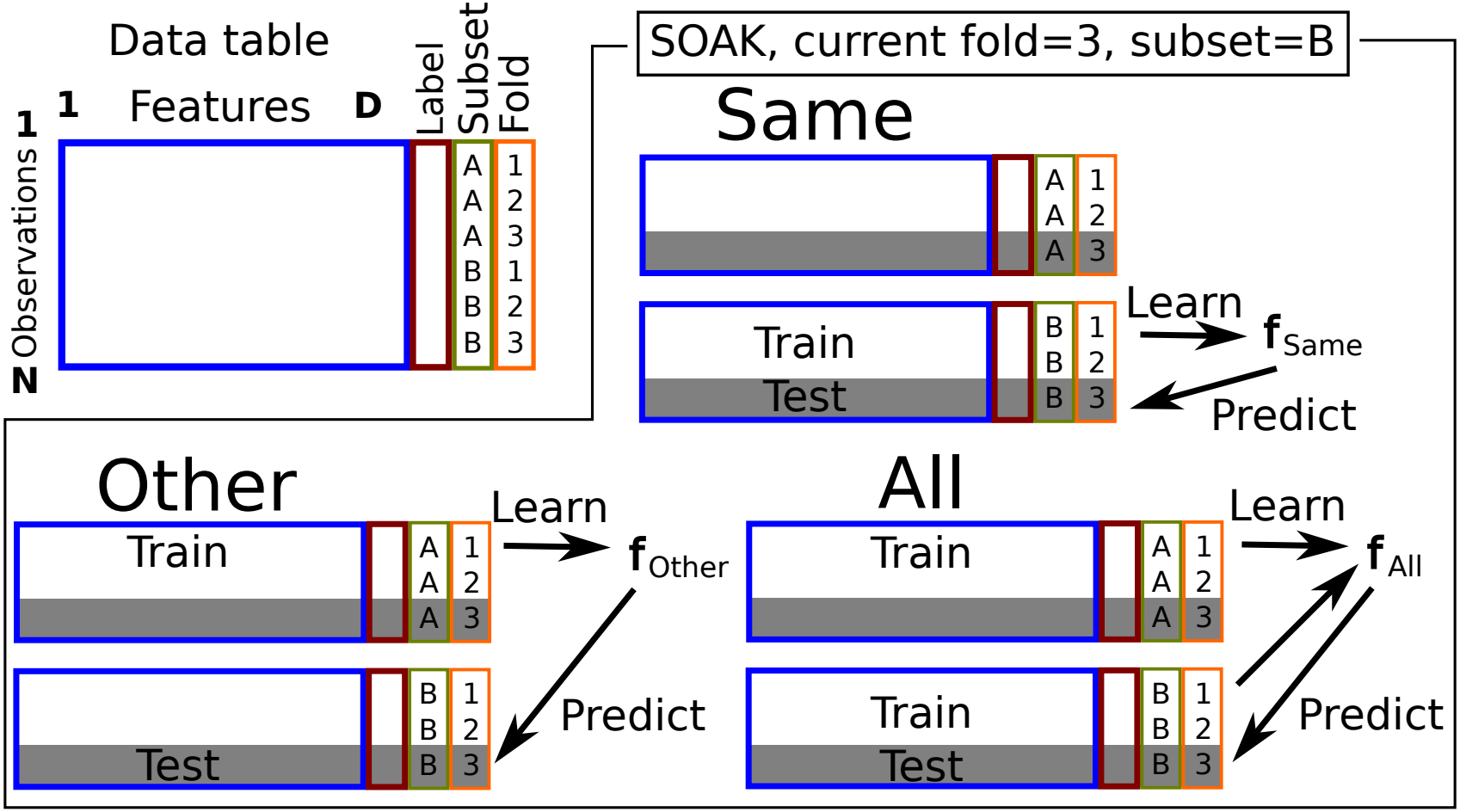
Proposed SOAK algorithm (Autism data example)

- Repeat for each test subset (2019,2020).



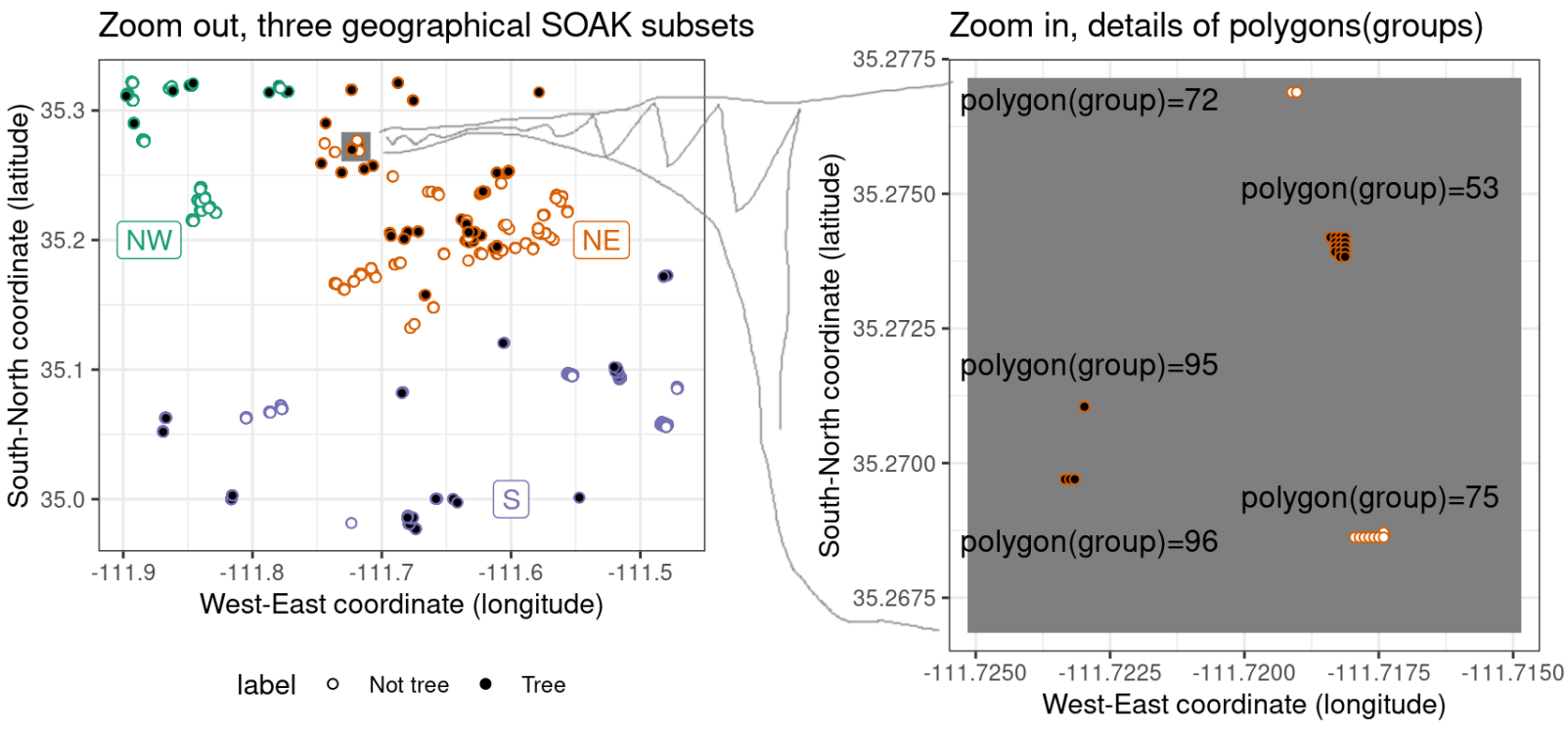
Proposed SOAK algorithm (generic data)

- Key new idea is **subset** column in data table.
- Compute test error for each subset (A/B) and fold (1/2/3).



Proposed SOAK algorithm is new/unique

- 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, interpretation/expectations

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

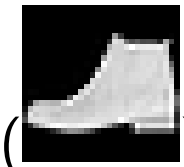
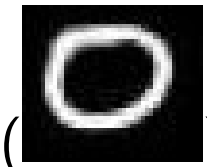
- **All** should be most accurate.
- **Same/Other** should be less accurate, because there is less data available (if other is larger than same, then other should be more accurate than same, etc).

If train/test are different (not iid),

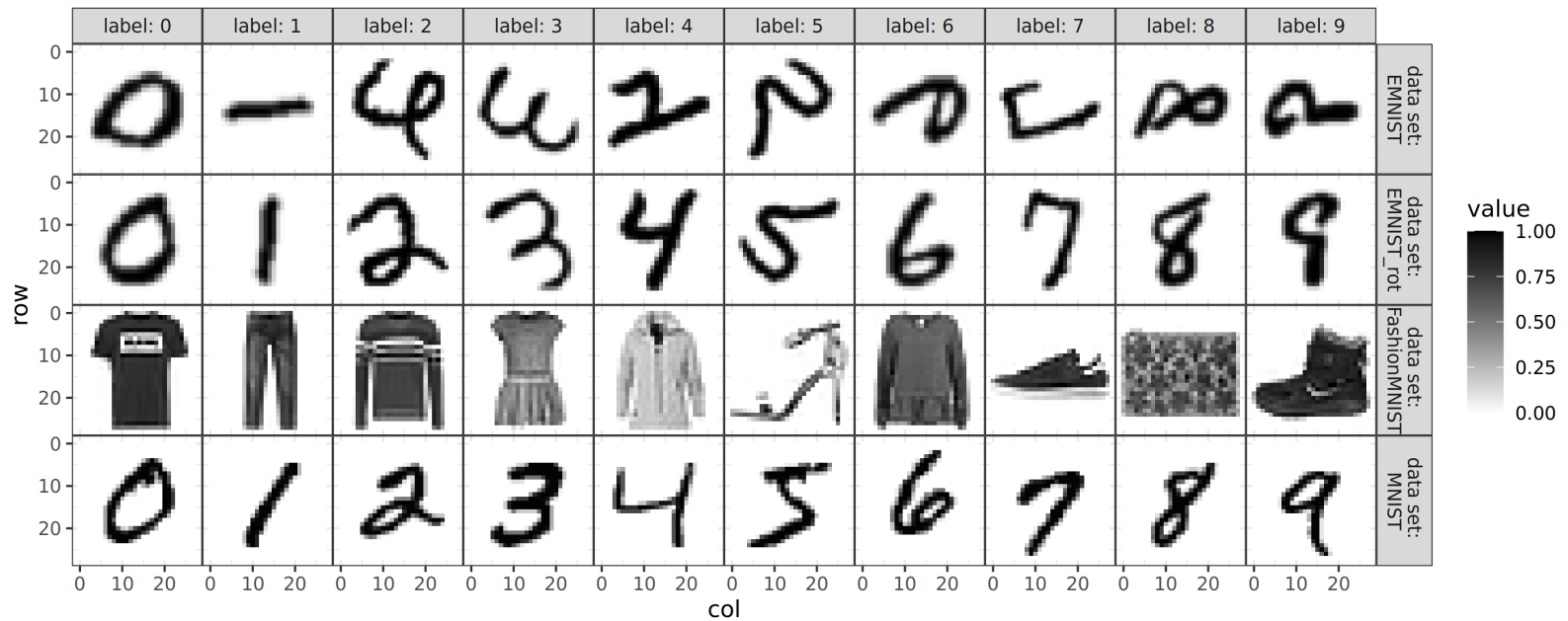
- **Same** should be most accurate.
- **Other** should be substantially less accurate.
- **All** accuracy should be between same and other.

- Can we train on one year, and accurately predict on another? Compare Same/Other test error.
- Can we get a more accurate model by combining data from different years? Compare Same/All test error.

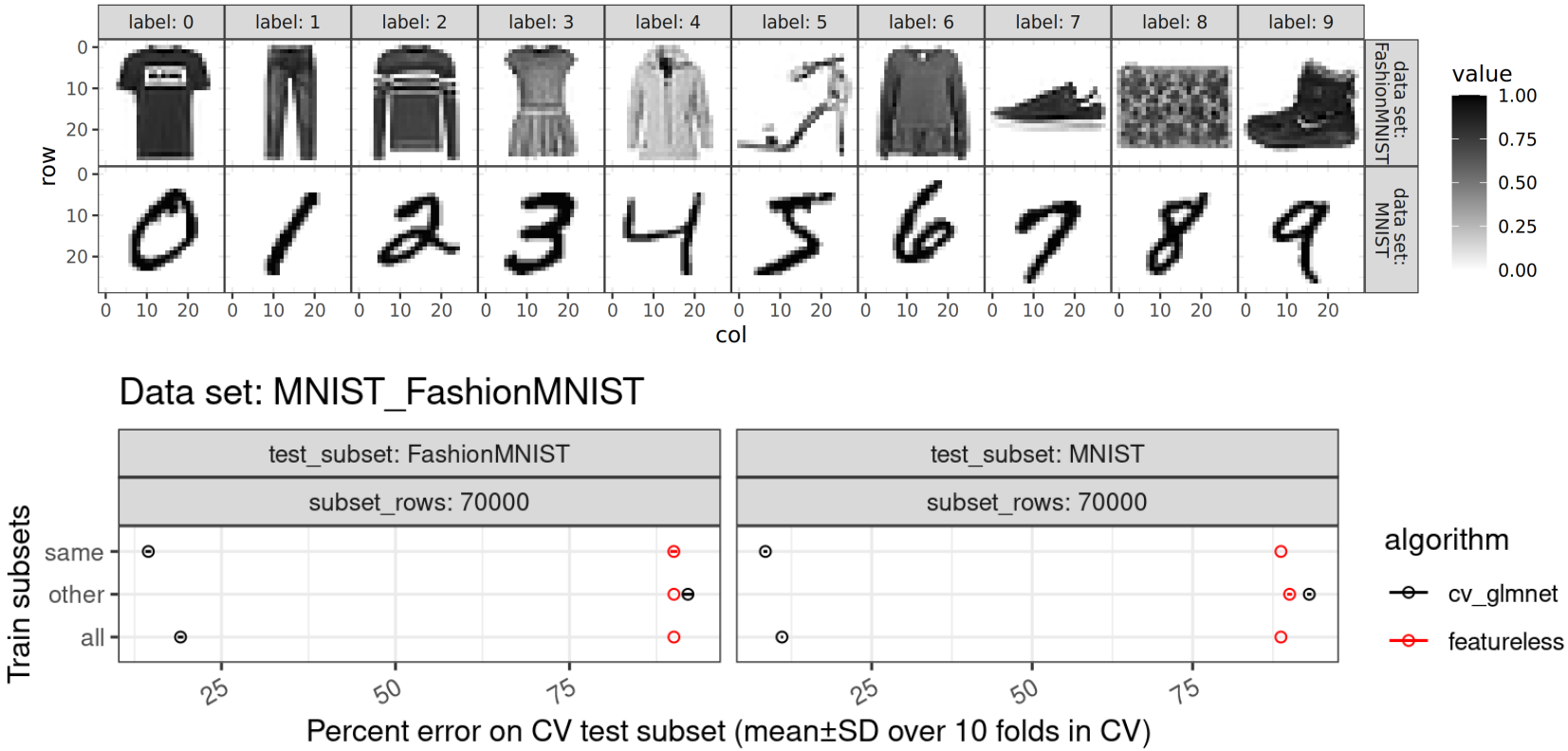
ImagePair data: train on MNIST and accurately predict on MNIST variants?

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

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

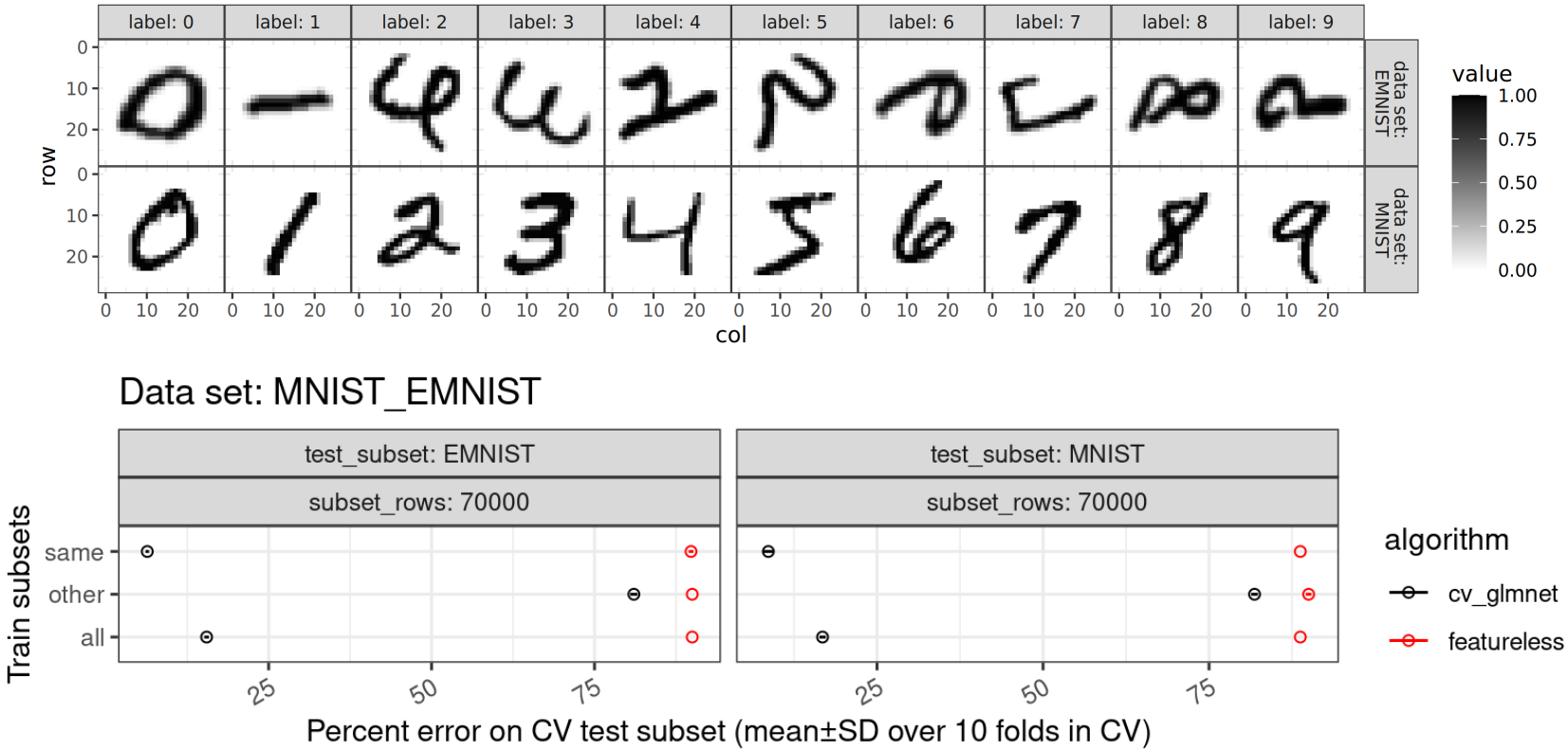


SOAK for MNIST+FashionMNIST data



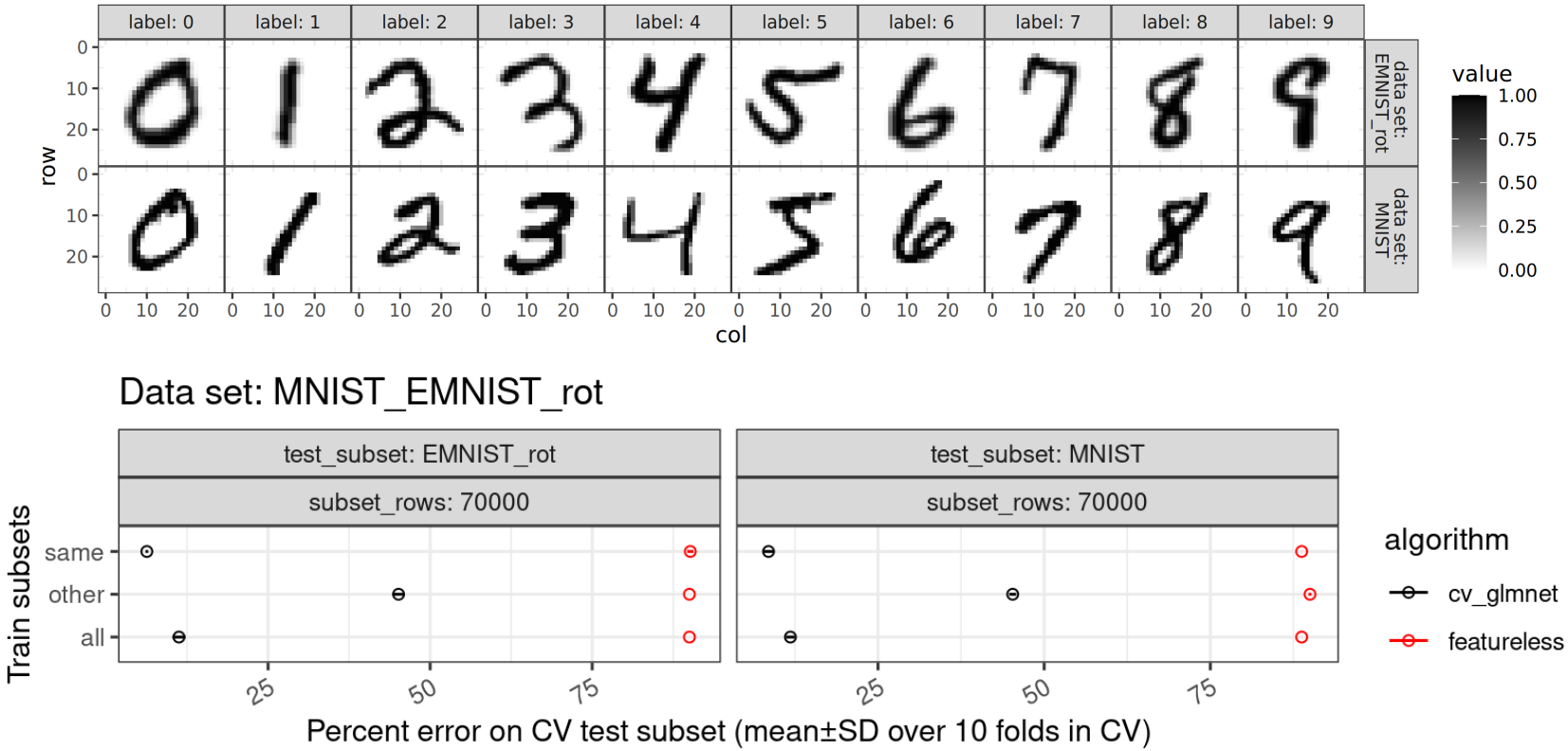
- Other linear model has greater test error than featureless, which indicates that the patterns are too different to learn anything at all.

SOAK for MNIST+EMNIST data



- Other has somewhat smaller test error than featureless, so something is learned/transferable between data sets, but it is still clear that the pattern is very different.

SOAK for MNIST+EMNIST_rot data

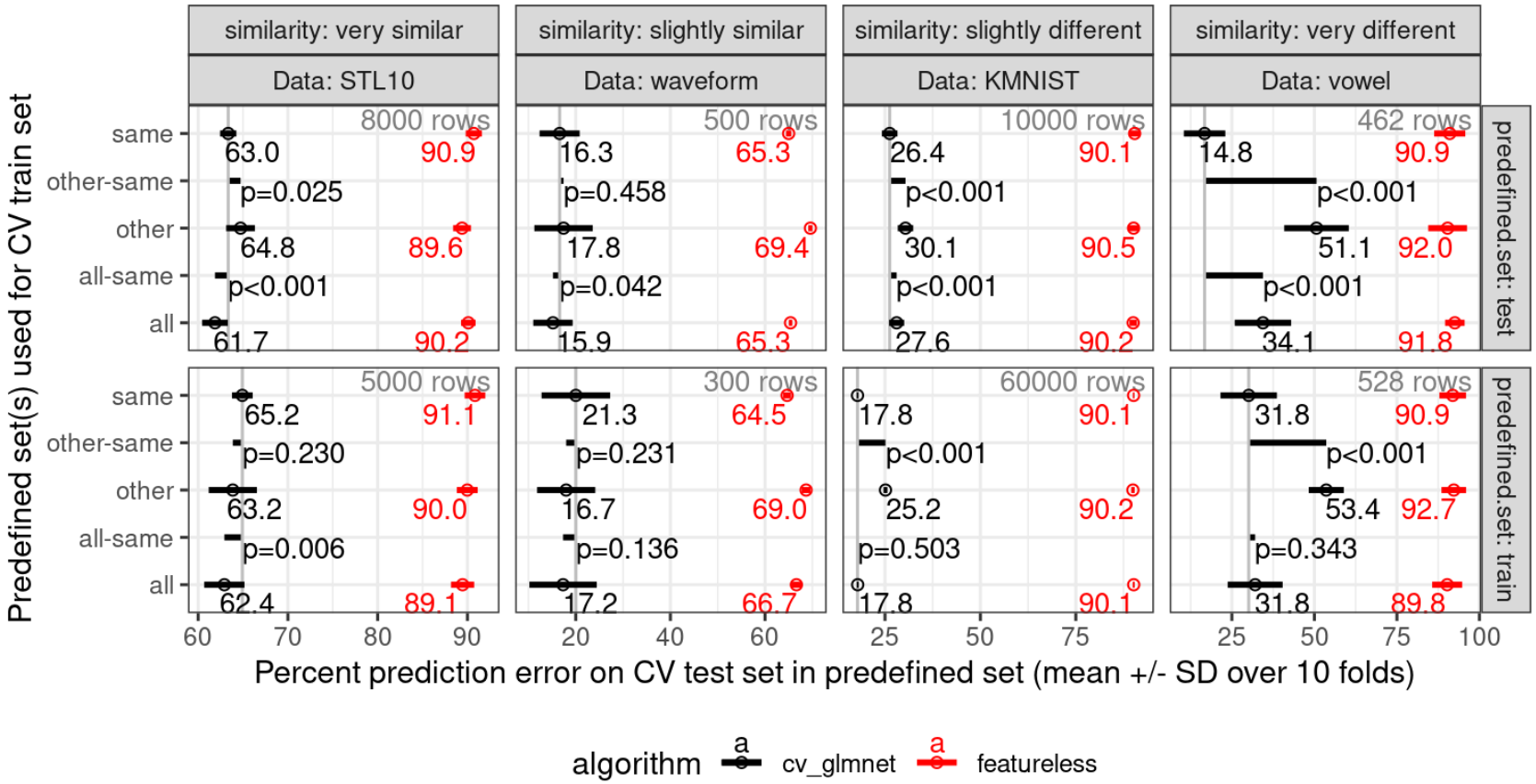


- Other still has larger test error than same, indicating some similarity between MNIST and EMNIST_rot data sets.

Benchmark data with a pre-defined train/test split

- 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?

Benchmark data with a pre-defined train/test split

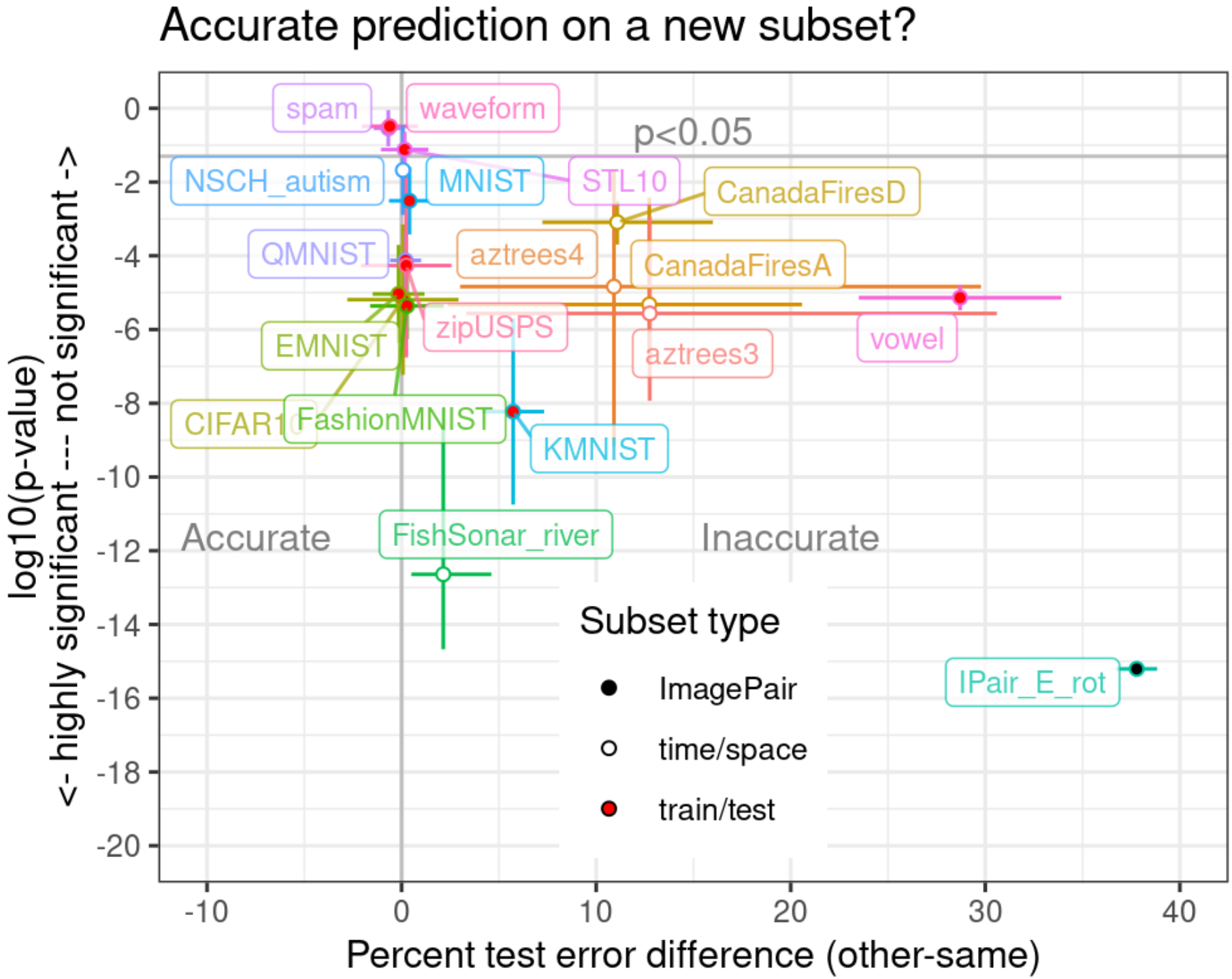


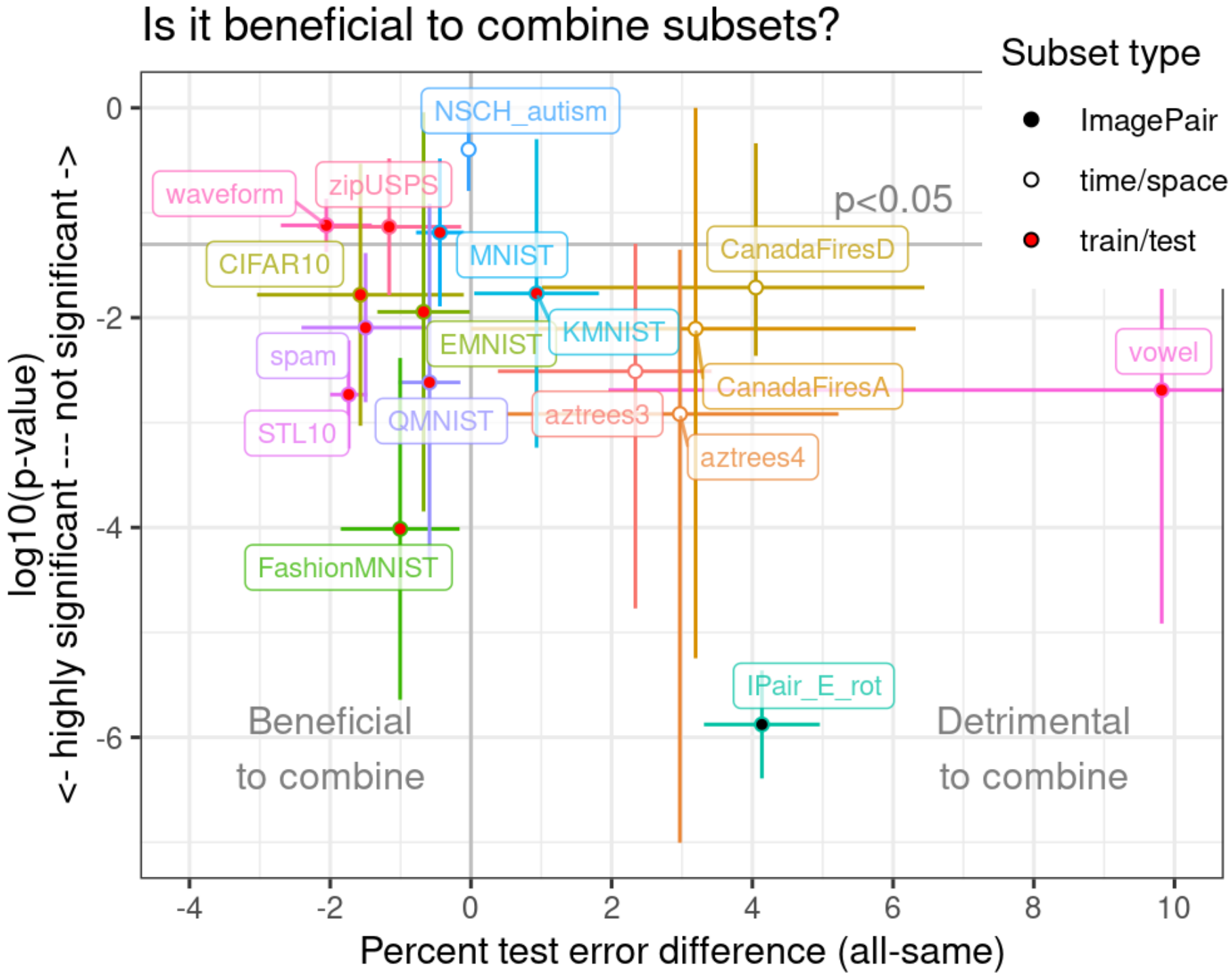
- Use pre-defined split as SOAK subset, to see if patterns are learnable/predictable in different pre-defined subsets.
- Left, similar subsets, all error less than same. (expected)
- Right, different subsets, all error greater than same. (surprising)

Data sets analyzed

- Sorted by test error difference between all and same.
- Different groups on top/positive.
- Similar groups on bottom/negative.

	data.name	rows	features	classes	n.groups	all-same
1	vowel	990	10	11	2	9.98
2	CanadaFires_downSampled	1491	46	2	4	4.02
3	CanadaFires_all	4827	46	2	4	3.39
4	aztrees4	5956	21	2	4	2.28
5	aztrees3	5956	21	2	3	2.05
6	FishSonar_river	2815744	81	2	4	1.69
7	KMNIST	70000	784	10	2	0.87
8	NSCH_autism	46010	364	2	2	-0.03
9	MNIST	70000	784	10	2	-0.53
10	QMNIST	120000	784	10	2	-0.70
11	spam	4601	57	2	2	-0.77
12	EMNIST	70000	784	10	2	-0.85
13	FashionMNIST	70000	784	10	2	-0.97
14	zipUSPS	9298	256	10	2	-1.44
15	waveform	800	21	3	2	-1.54
16	CIFAR10	60000	3072	10	2	-1.77
17	STL10	13000	27648	10	2	-1.97


Accurate prediction on a new subset?
spam
waveform
p<0.05
NSCH_autism
MNIST
STL10
CanadaFiresD
QMNIST
aztrees4
CanadaFiresA
zipUSPS
vowel
EMNIST
aztrees3
CIFAR1
FashionMNIST
KMNIST
Accurate
FishSonar_river
Inaccurate
Subset type
ImagePair
time/space
train/test
IPair_E_rot
log10(p-value)
<- highly significant --- not significant ->
0
-2
-4
-6
-8
-10
-12
-14
-16
-18
-20
-10
0
10
20
30
40
Percent test error difference (other-same)


Is it beneficial to combine subsets?
Subset type
ImagePair
time/space
train/test
p<0.05
NSCH_autism
waveform
zipUSPS
MNIST
CIFAR10
CanadaFiresD
KMNIST
EMNIST
spam
vowel
CanadaFiresA
QMNIST
aztrees3
STL10
aztrees4
FashionMNIST
IPair_E_rot
Beneficial
to combine
Detrimental
to combine
log10(p-value)
<- highly significant --- not significant ->
0
-2
-4
-6
-4
-2
0
2
4
6
8
10
Percent test error difference (all-same)

Discussion and Conclusions

- Proposed SOAK algorithm shows if data subsets are similar enough for learning/prediction.
- In Autism data, there was a slight benefit to combining years.
- In fires/trees/fish data, we observed significant differences between images/regions/rivers.
- Some pre-defined train/test splits in benchmark data are similar/iid (STL10/waveform), others are not (KMNIST/vowel).
- Free/open-source R package available in mlr3 framework (easy parallelization over algorithms, train/test splits, data sets) `https://github.com/tdhock/mlr3resampling`
- These slides are reproducible, using the code in `https://github.com/tdhock/cv-same-other-paper`

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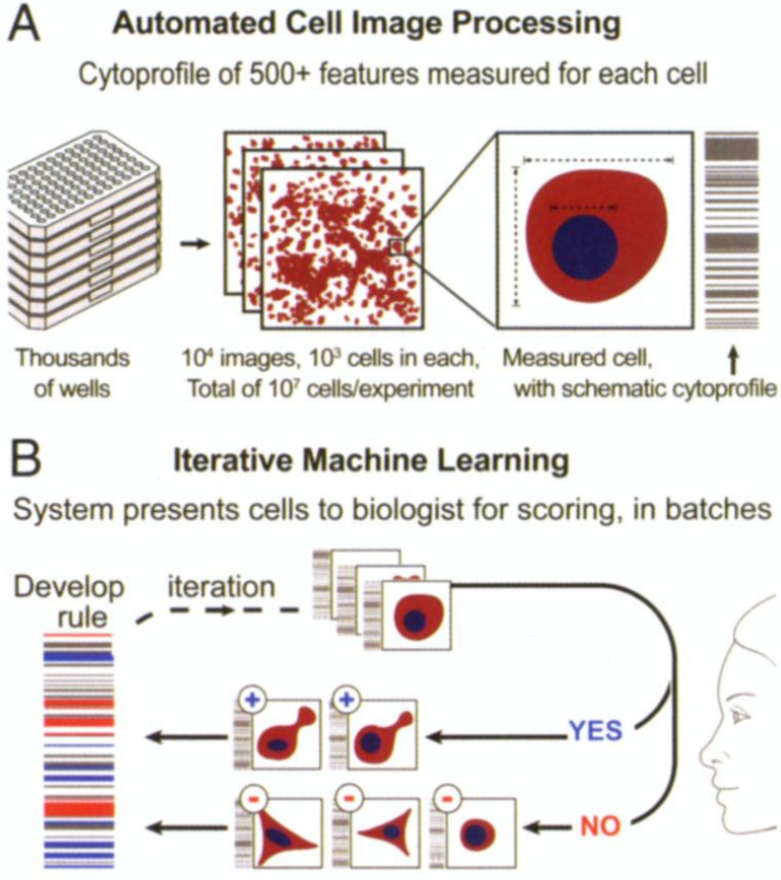
AUM=Area Under Min(FPR,FNR), a new differentiable loss for ROC curve optimization

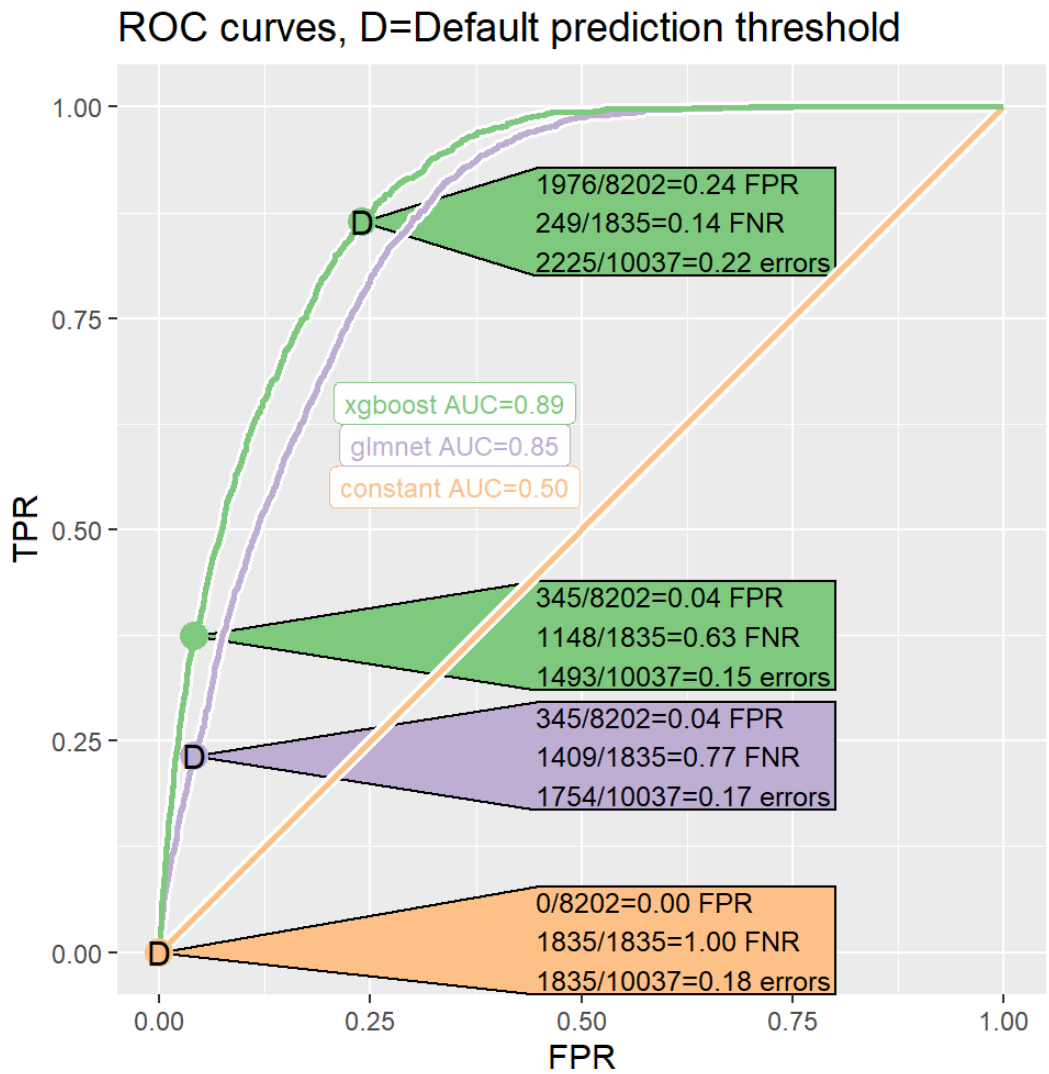
Problem: supervised binary classification

- 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.



Most algorithms (SVM, Logistic regression, 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).

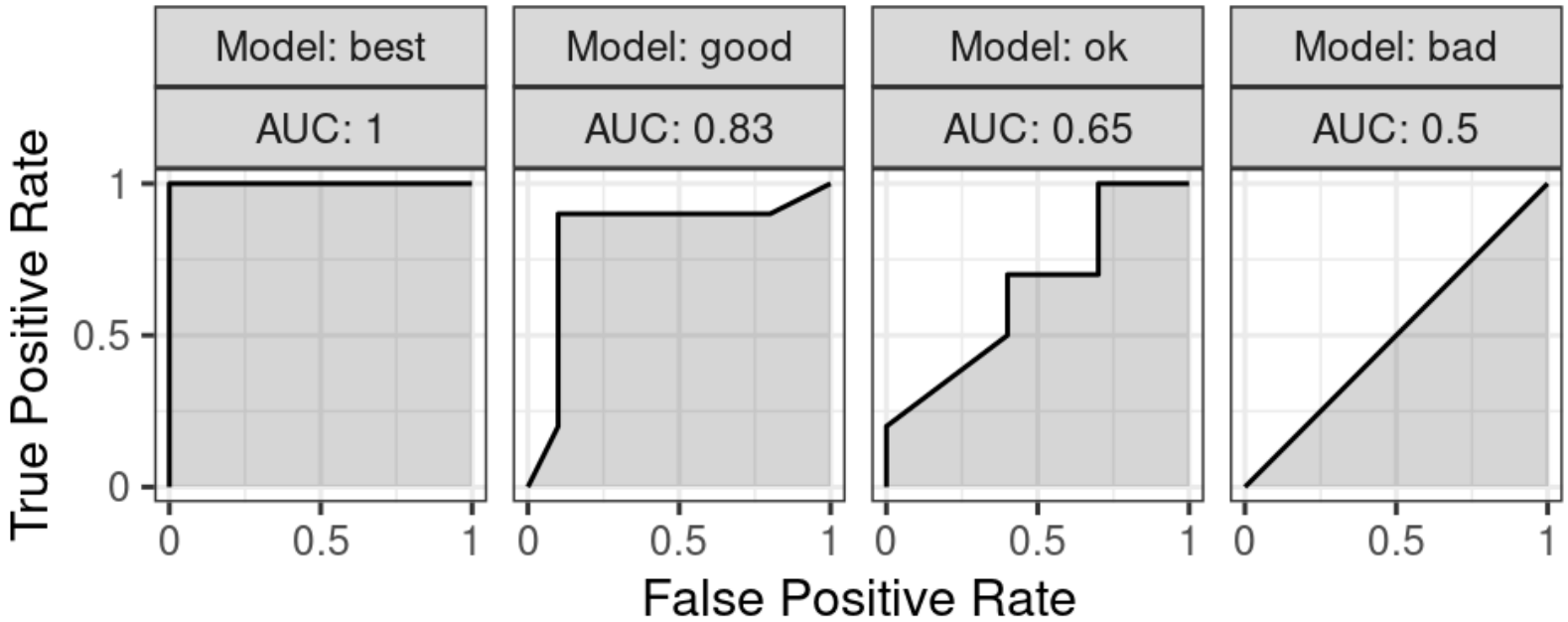
ROC curves for evaluation, especially useful with imbalance



- At default FPR=24% (D), glmnet has fewer errors.
- At FPR=4%, xgboost has fewer errors.

Receiver Operating Characteristic (ROC) Curves

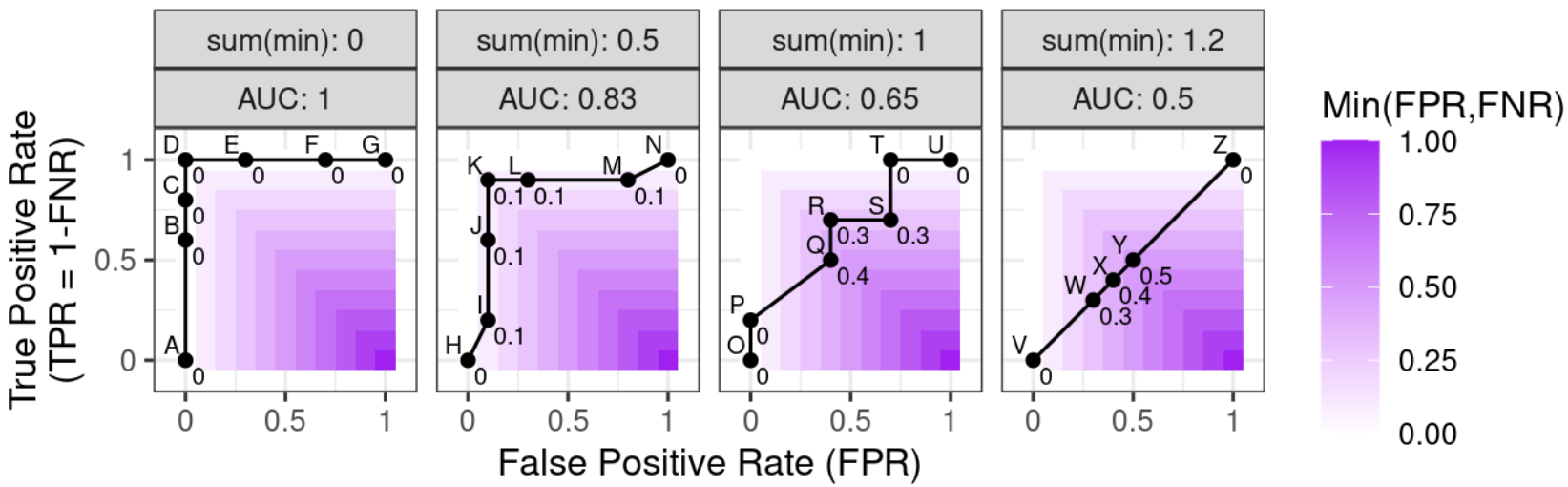
- Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- ROC curve of learned f is plot of True Positive Rate vs False Positive Rate: each point on the ROC curve is a different constant $c \in \mathbb{R}$ added to the predicted values: $f(\mathbf{x}) + c$.
- $c = \infty$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



Research question and new idea

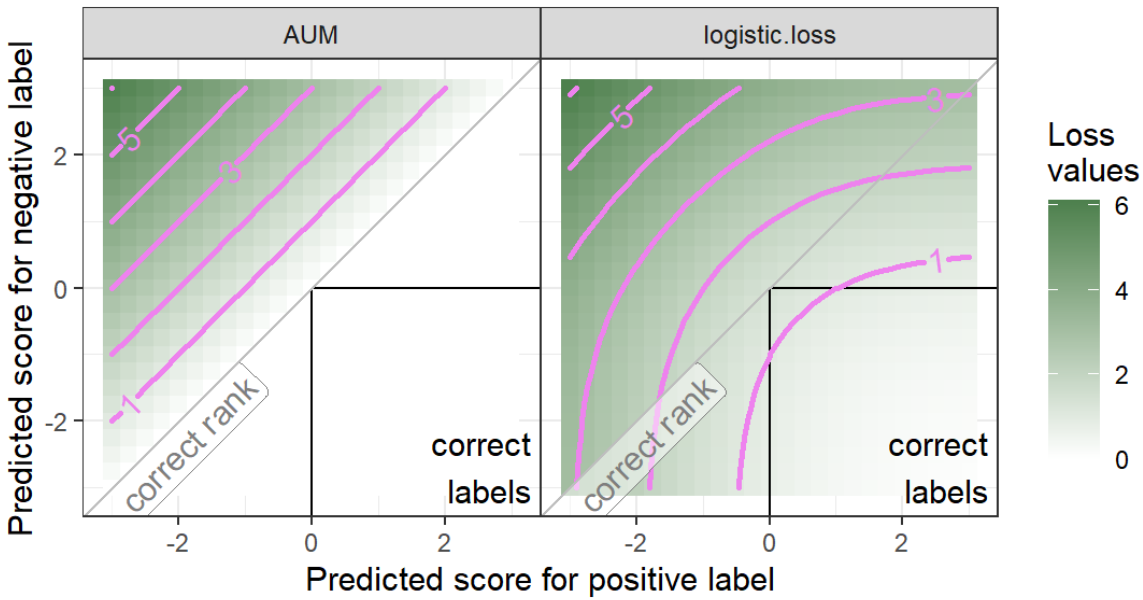
Can we learn a binary classification function f which directly optimizes the ROC curve?

- 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(FPR,FNR).



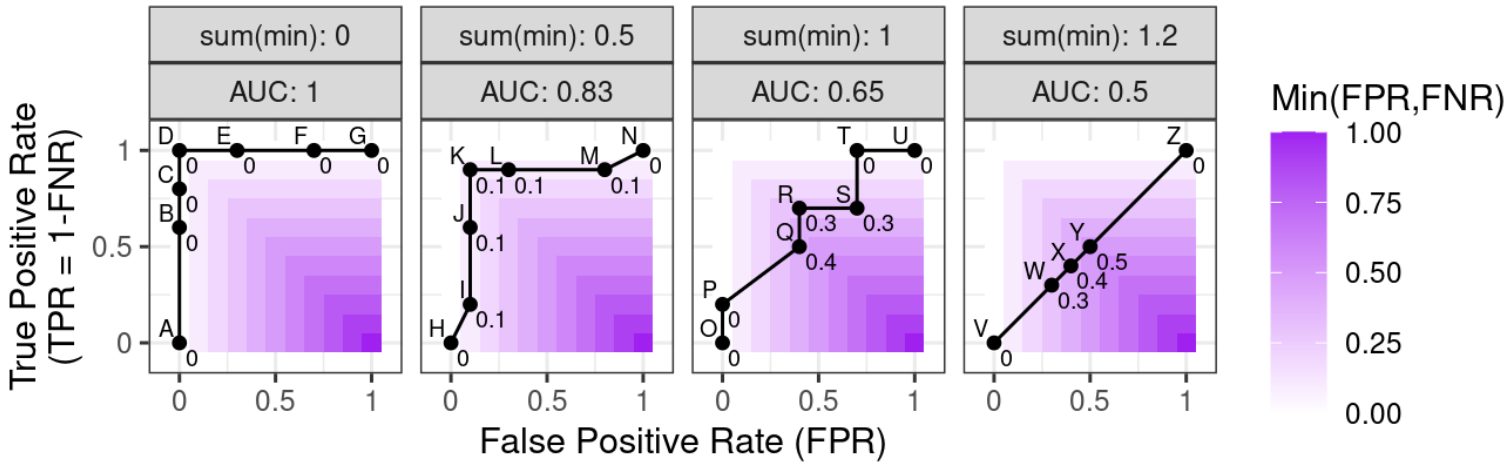
Comparing proposed loss with baselines

- 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$^{\text{struct}}$ (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.

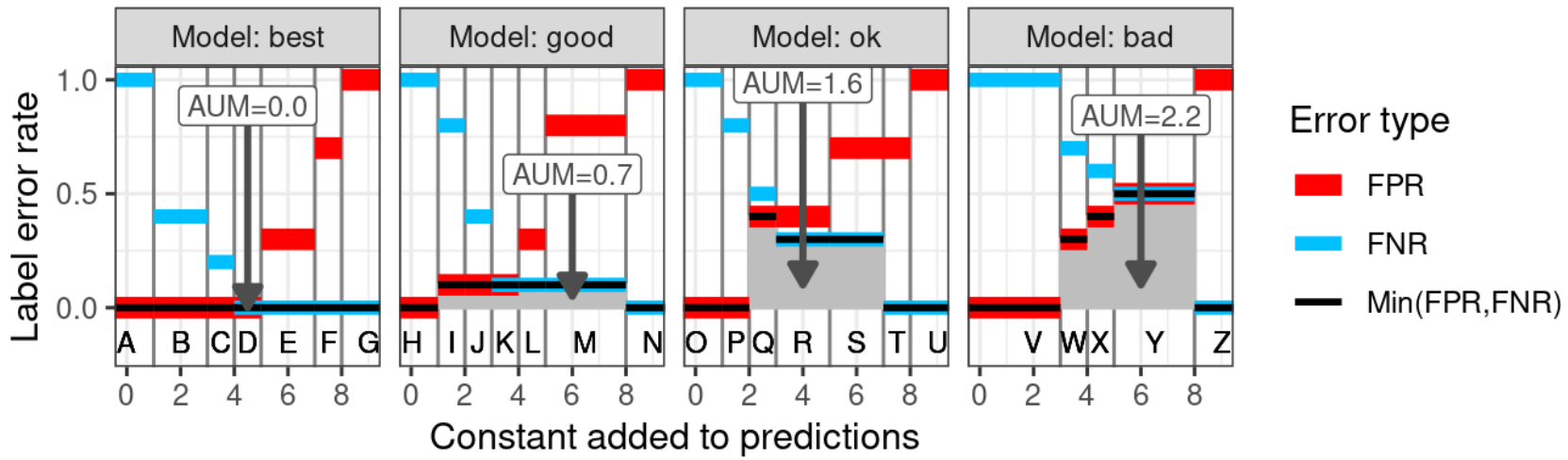


Barr, Hocking, Morton, Thatcher, Shaw, *TransAI* (2022).

Large AUC ≈ small Area Under Min(FP,FN) (AUM)

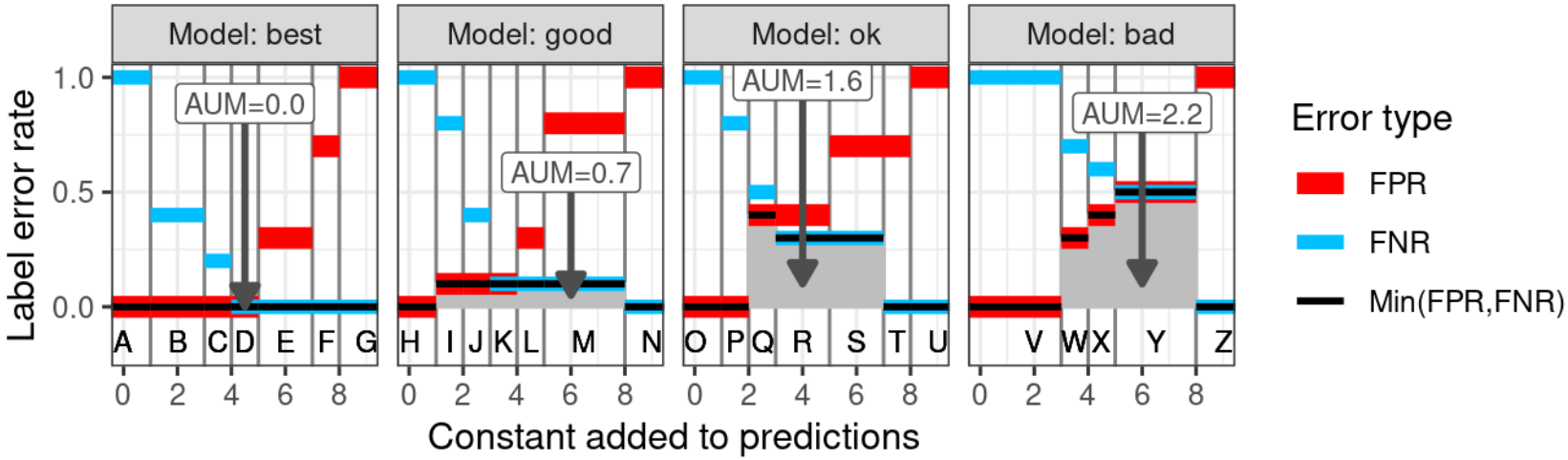


Above: purple heat map = numbers near dots = distance to top or left = same as black min error rate functions below.



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

Computing Sum of Min (SM)

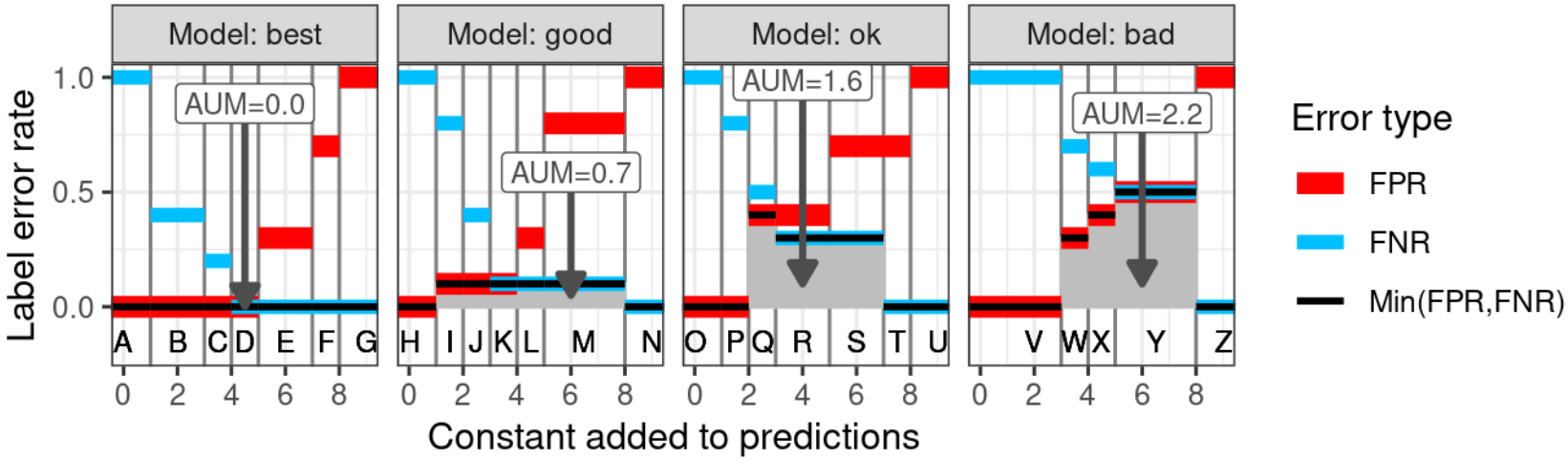


- For N samples, there are $\leq N+1$ points on the ROC curve,
- with sorted thresholds $T_1 \leq \cdots \leq T_N \in \mathbb{R}$,
- and corresponding min error values $M_1, \ldots, M_N$.
- Then if I is the indicator function, we can write the sum of the min (SM), over all ROC points, as:

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

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

Computing Area Under Min (AUM)



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

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

$$\text{AUM} = \sum_{i=2}^{N} [T_i - T_{i-1}] M_i.$$

AUM is therefore a surrogate loss for ROC optimization, and it is differentiable almost everywhere $\Rightarrow$ gradient descent learning!

ROC curve pytorch code

```
def ROC_curve(pred_tensor, label_tensor):
    sorted_indices = torch.argsort(-pred_tensor)
    ...
    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])])
    }
```

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

AUC and AUM pytorch code uses argsort

- ROC AUC and proposed AUM are both implemented by first computing the ROC curve.

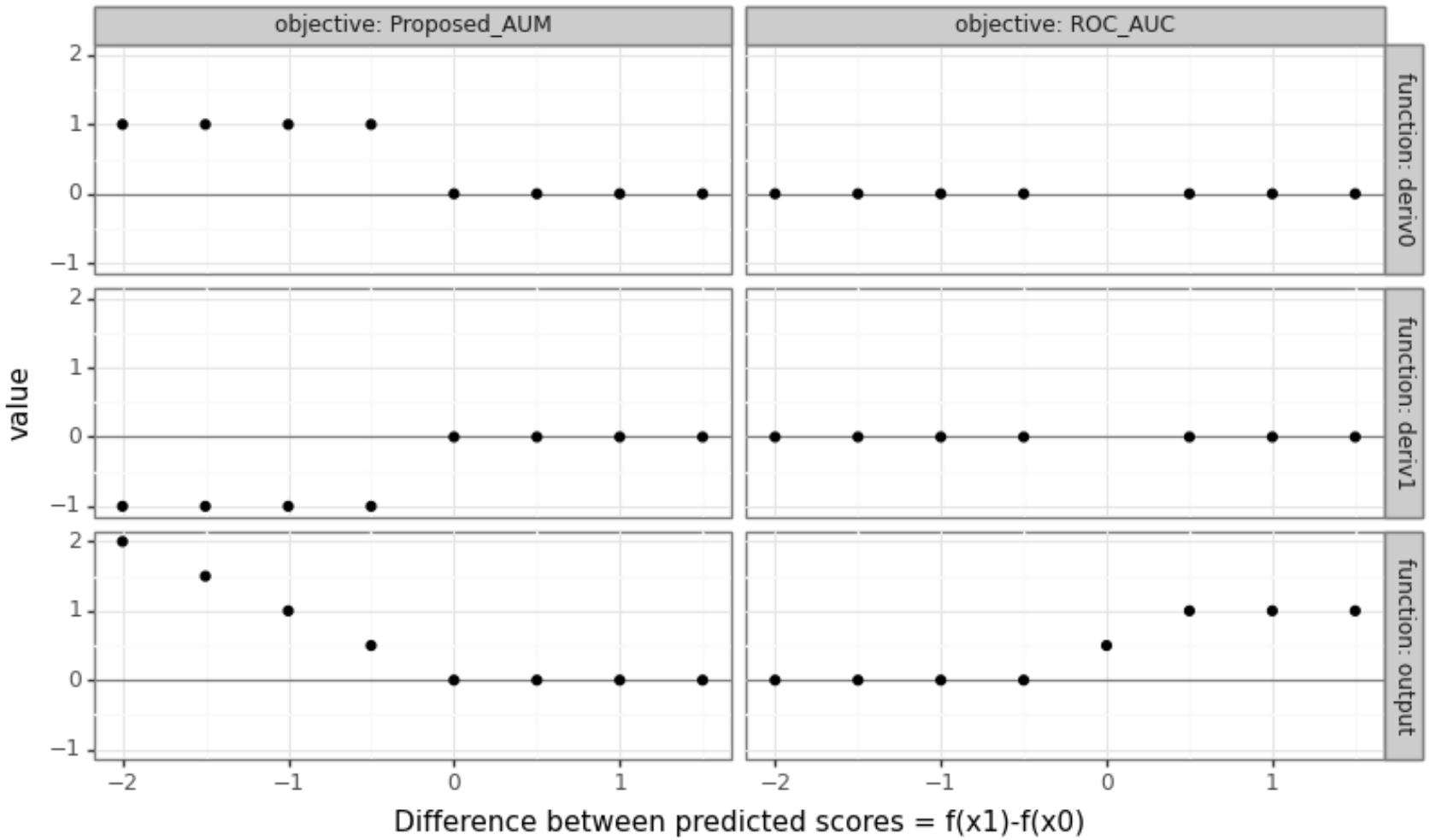
```
def ROC_AUC(pred_tensor, label_tensor):
    roc = ROC_curve(pred_tensor, label_tensor)
    FPR_diff = roc["FPR"][1:]-roc["FPR"][:-1]
    TPR_sum = roc["TPR"][1:]+roc["TPR"][:-1]
    return torch.sum(FPR_diff*TPR_sum/2.0)

def Proposed_AUM(pred_tensor, label_tensor):
    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/

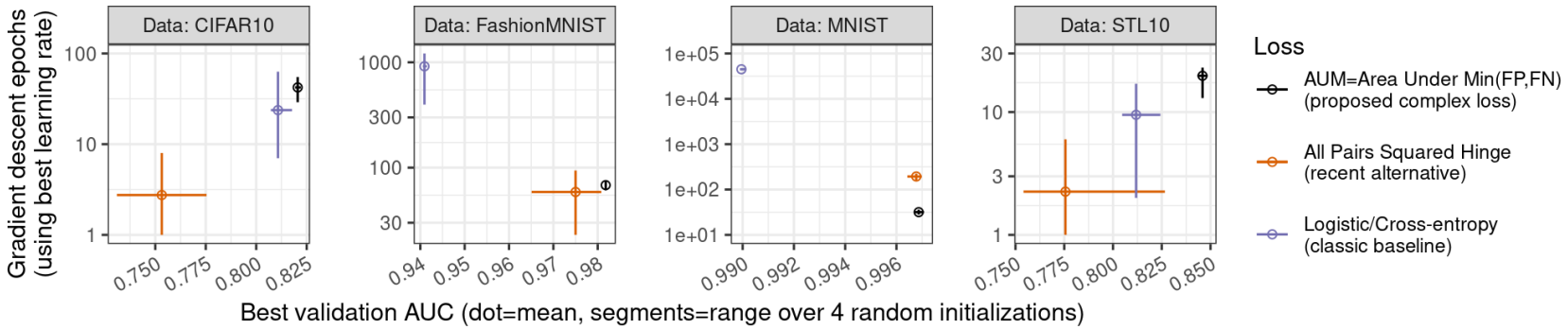
AUM pytorch code, auto-grad demo

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



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

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 (like LibAUC/X-risk).
- Number of epochs comparable to baselines.
- 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 baselines are simple (sum over samples).
- Proposed AUM loss similar to recent losses that sum over all pairs of positive and negative examples (both can be implemented by sorting predicted scores)
- Proposed AUM loss uses a different/novel relaxation.
- Proposed AUM loss implemented in pytorch code, can be used as a drop-in replacement for logistic/binary cross-entropy loss, `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.
- Margin-based algorithms like SVM?
- Works well in binary classification, how to adapt to multi-class setting, or other problems such as ranking/information retrieval? (see our JMLR'23 paper for an application to change-point detection, and arXiv:2410.08635 for an efficient line search that exploits the piecewise linear/constant nature of AUM/AUC)

Thanks to my students and collaborators!

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