Efficient line search optimization of penalty functions in supervised changepoint detection

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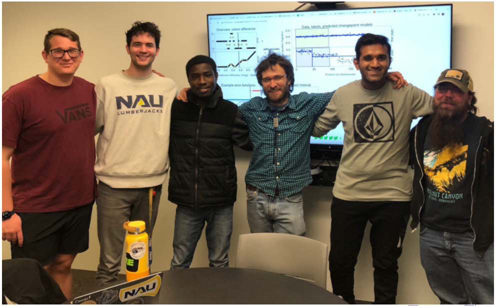


Problem Setting 1: ROC curves for evaluating supervised binary classification algorithms

Problem setting 2: ROC curves for evaluating supervised changepoint algorithms

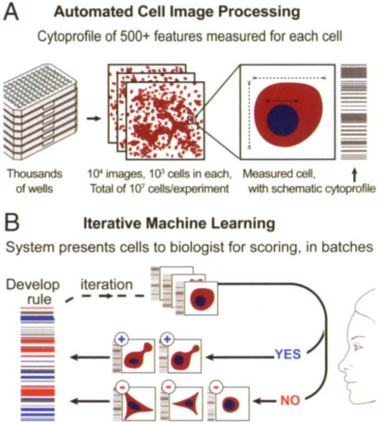
Proposed line search algorithm for surrogate loss: Area Under Min{FP,FN} (AUM)

Empirical results: increased speed and accuracy using proposed line search

Discussion and Conclusions

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.



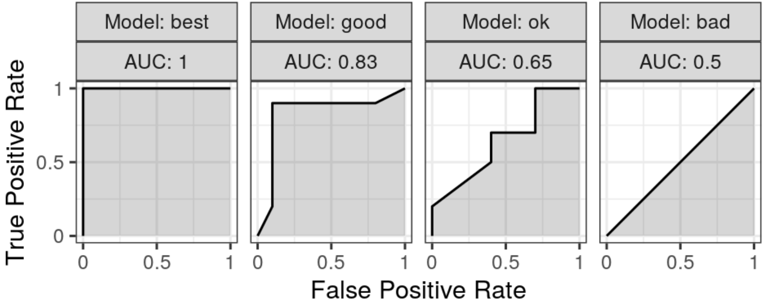
Most algorithms (SVM, Logistic regression, etc) minimize a differentiable surrogate of zero-one loss = sum of:

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).

Receiver Operating Characteristic (ROC) Curves

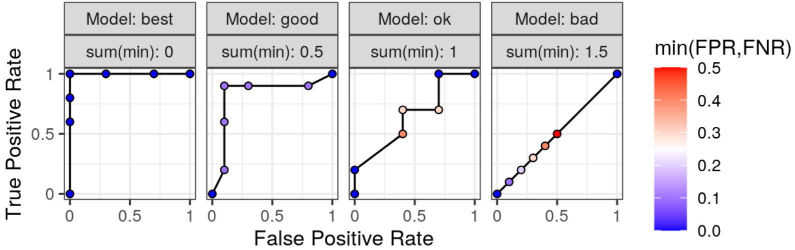
- Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- For a given set of predicted scores, plot True Positive Rate vs False Positive Rate, each point on the ROC curve is a different threshold of the predicted scores.
- Best classifier has a point near upper left (TPR=1, 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 propose 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(FP,FN).



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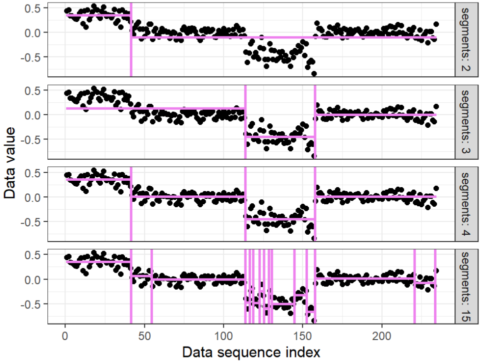
Problem: unsupervised changepoint detection

- Data sequence $z_1, \dots, z_T$ at T points over time/space.
- Ex: DNA copy number data for cancer diagnosis, $z_t \in \mathbb{R}$.
- The penalized changepoint problem (Maidstone *et al.* 2017)

$$\arg\min_{u_1,\dots,u_T \in \mathbb{R}} \sum_{t=1}^{T} (u_t - z_t)^2 + \lambda \sum_{t=2}^{T} I[u_{t-1} \neq u_t].$$

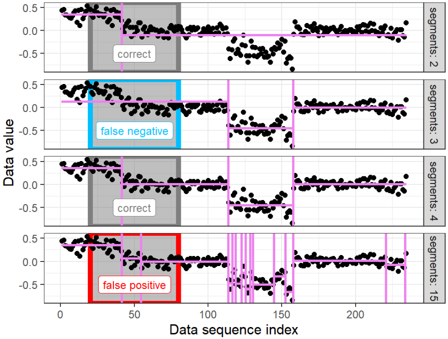


Larger penalty λ results in fewer changes/segments.

Smaller penalty λ results in more changes/segments.

Problem: weakly supervised changepoint detection

- First described by Hocking *et al.* ICML 2013.
- We are given a data sequence $\mathbf{z}$ with labeled regions L.
- We compute features $\mathbf{x} = \phi(\mathbf{z}) \in \mathbf{R}^p$ and want to learn a function $f(\mathbf{x}) = -\log \lambda \in \mathbf{R}$ that minimizes label error (sum of false positives and false negatives), or maximizes AUC.



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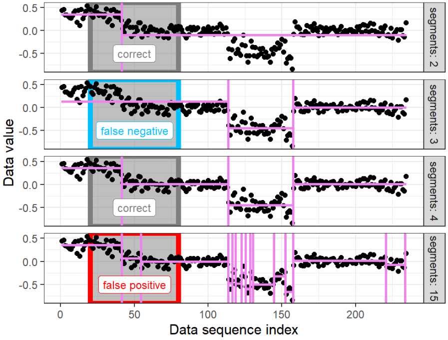
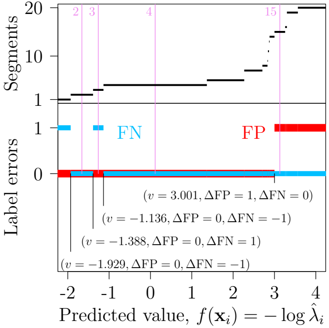
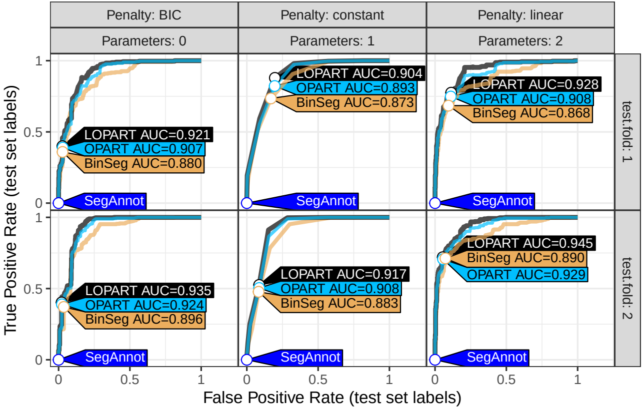




Comparing changepoint algorithms using ROC curves

Hocking TD, Srivastava A. Labeled Optimal Partitioning. Computational Statistics (2022).



LOPART algorithm (R package LOPART) has consistently larger test AUC than previous algorithms.

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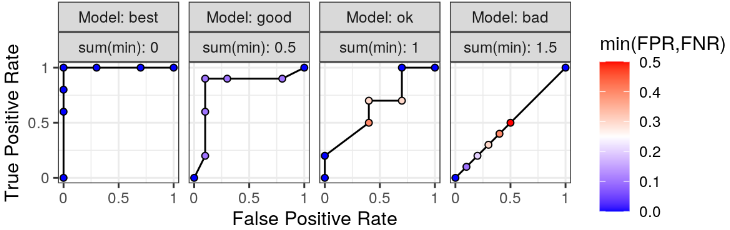
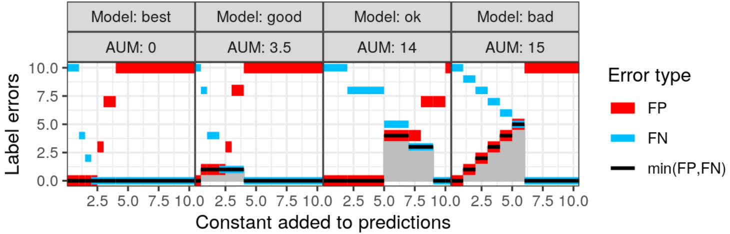
Large AUC ≈ small Area Under Min(FP,FN) (AUM)





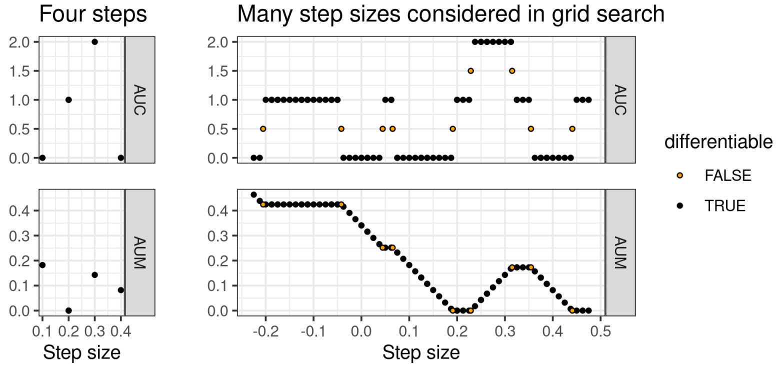
Hocking, Hillman, *Journal of Machine Learning Research* (2022).
Barr, Hocking, Morton, Thatcher, Shaw, *TransAI* (2022).

Proposed line search algorithm uses AUC/AUM structure

When learning a linear model,

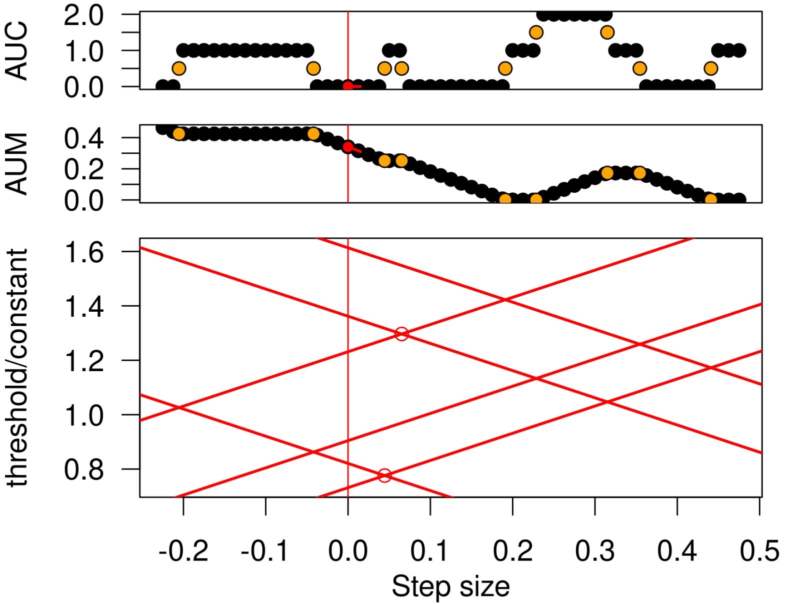
- AUC is piecewise constant, and
- AUM is piecewise linear,

as a function of step size in gradient descent.

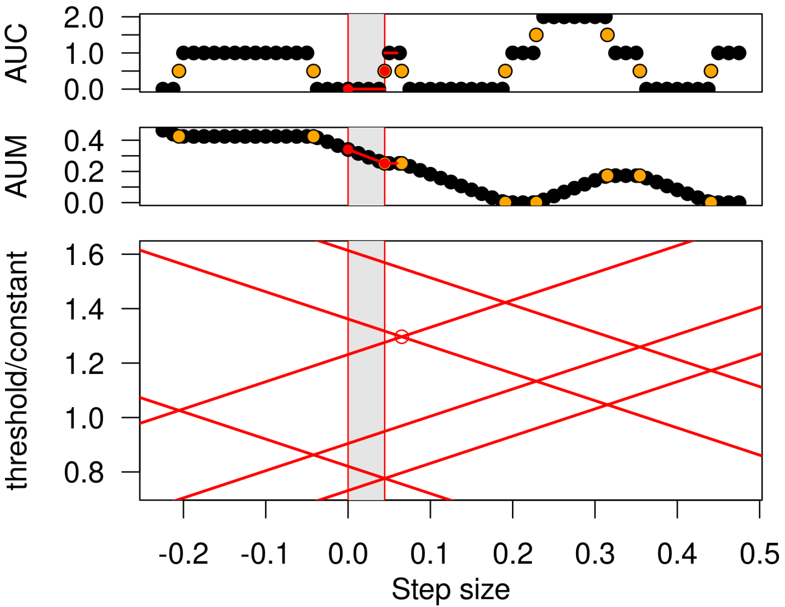


Proposed line search algorithm computes updates when there are possible changes in slope of AUM / values of AUC (orange dots).

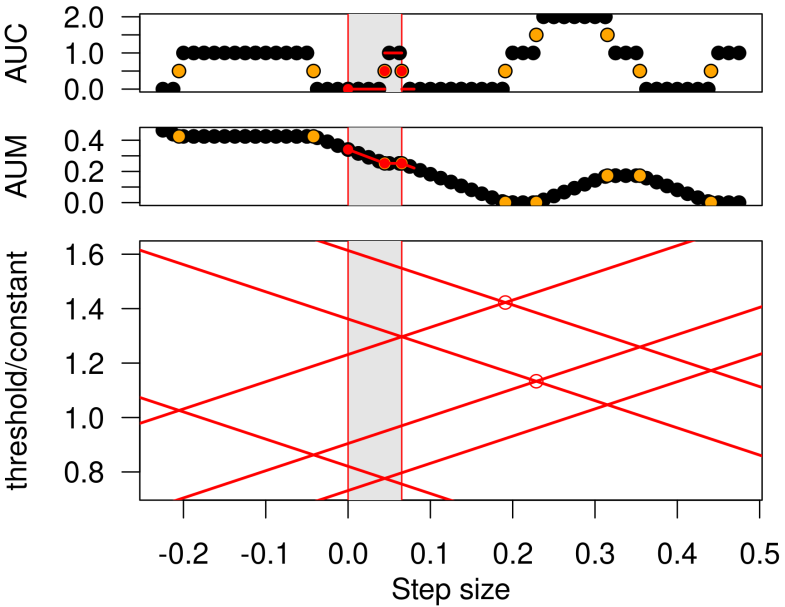
AUM/AUC line search, iteration 1



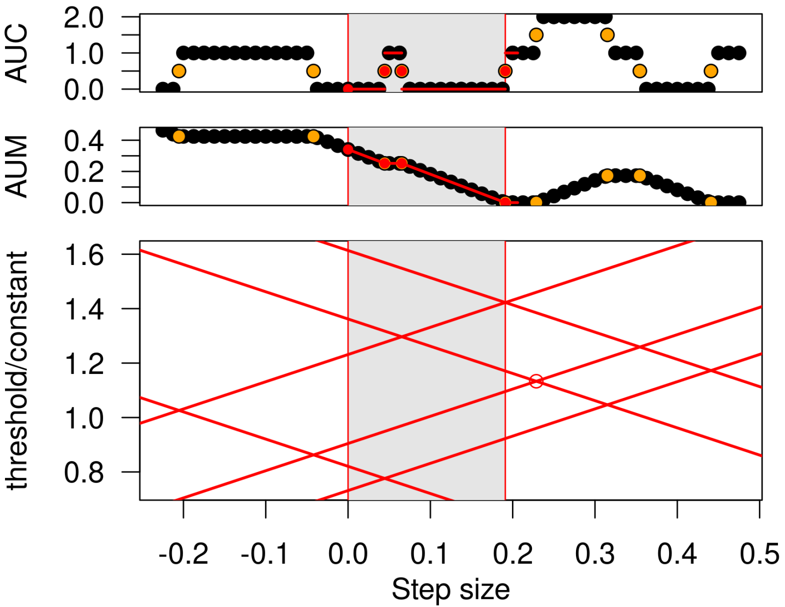
AUM/AUC line search, iteration 2



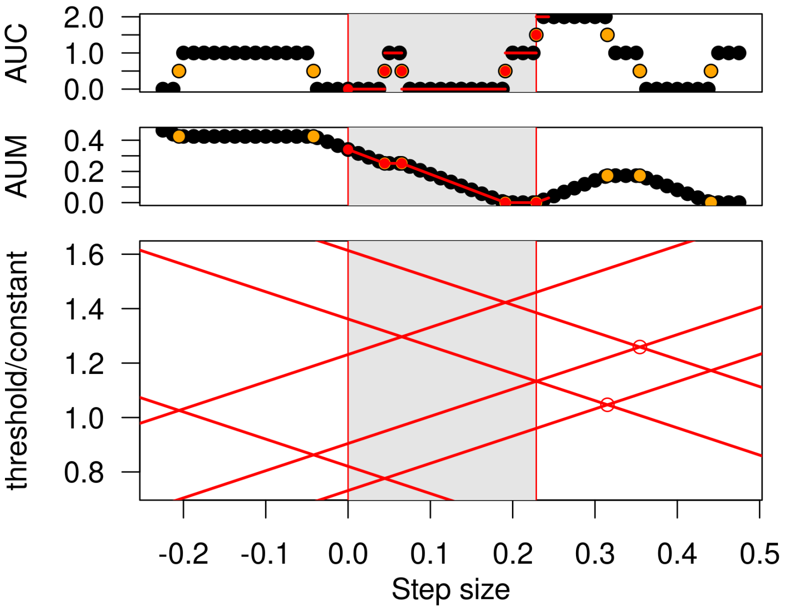
AUM/AUC line search, iteration 3



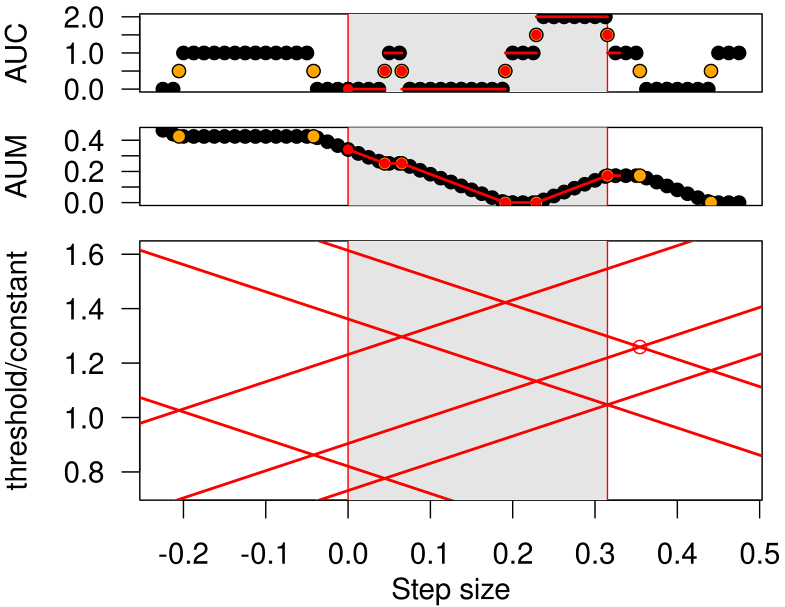
AUM/AUC line search, iteration 4



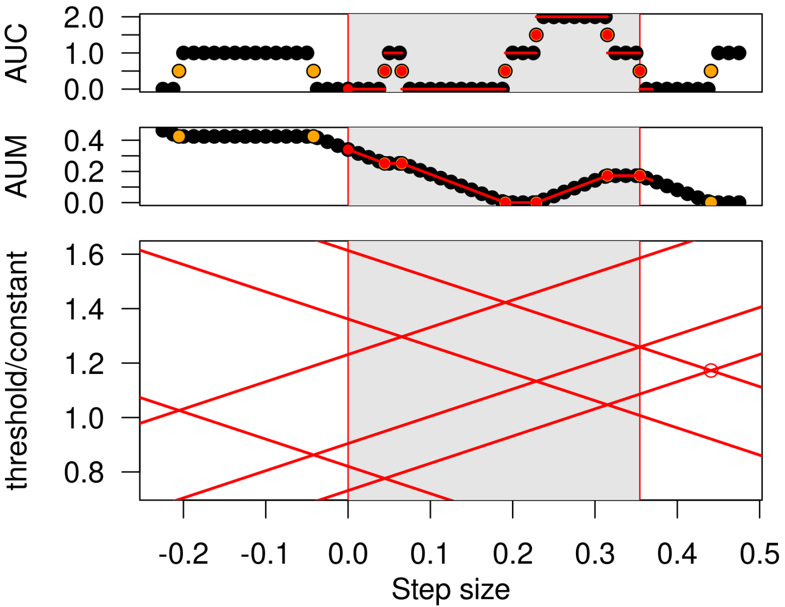
AUM/AUC line search, iteration 5



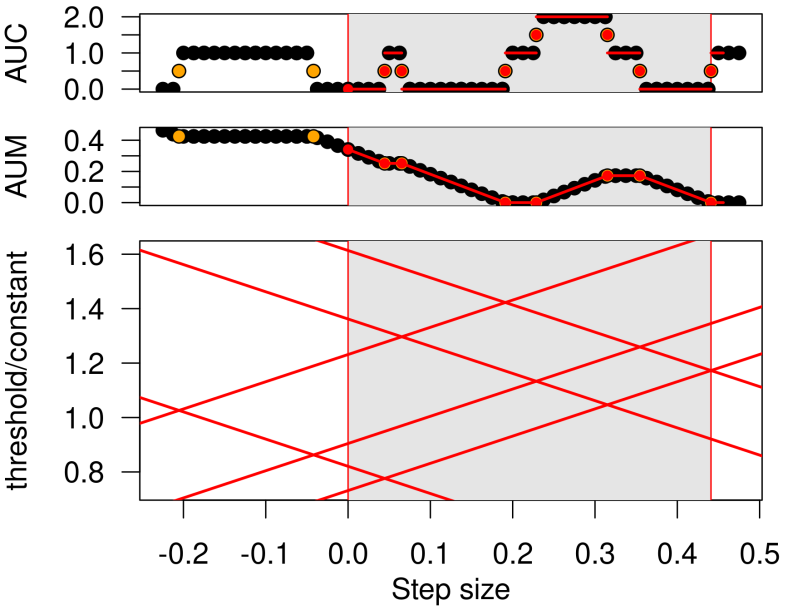
AUM/AUC line search, iteration 6



AUM/AUC line search, iteration 7



AUM/AUC line search, iteration 8



Complexity analysis of proposed algorithm

For N labeled observations, worst case $O(N)$ space, and

grid: standard grid search. Linear $O(N \log N)$ time, but potentially slow for a sub-optimal grid search.

exactL: only first N line search iterations. Linear $O(N \log N)$ time, relatively small step sizes chosen, relatively large number of steps overall in gradient descent.

exactQ: all line search iterations. Quadratic $O(N^2 \log N)$ time, large step sizes, small number of steps.

min.aum: keep doing line search iterations until first AUM increase. Same as exactQ time.

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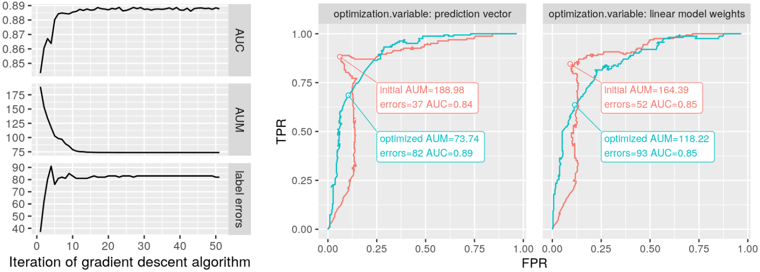
AUM gradient descent results in increased train AUC for a real changepoint problem

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



- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), gradient descent on weight vector.

Learning algorithm results in better TODO AUC/AUM for changepoint problems

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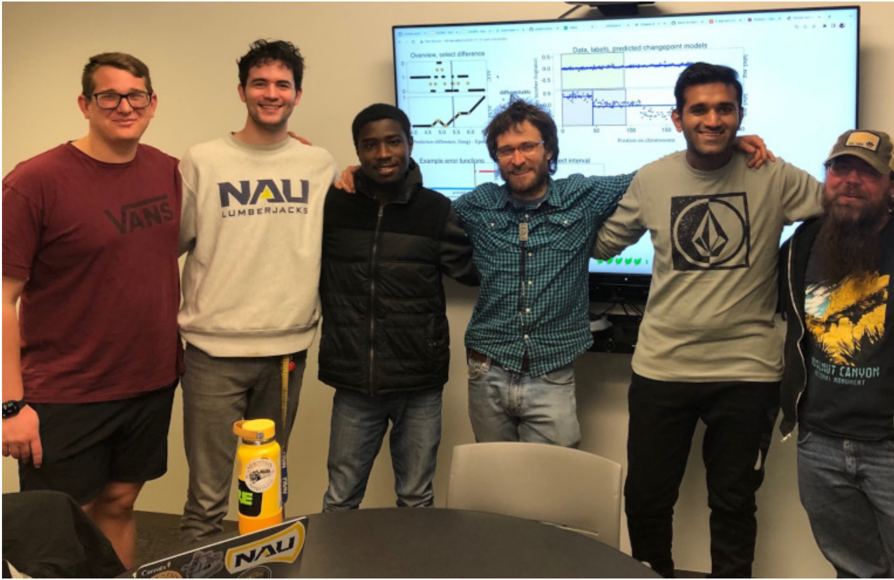
- ROC curves are used to evaluate binary classification and changepoint detection algorithms.
- A new loss function, AUM=Area Under Min(FP,FN), is a differentiable surrogate of the sum of Min(FP,FN) over all points on the ROC curve.
- We propose new gradient descent algorithm with efficient line search, for optimizing AUM/AUC.
- Implementations available in R/C++ and python:
  `https://cloud.r-project.org/web/packages/aum/` (R/C++ line search)
  `https://tdhock.github.io/blog/2022/aum-learning/` (pytorch AUM loss)
- Empirical results provide evidence that line search is faster and more accurate than grid search.
- Future work: non-linear learning algorithms that use AUM minimization as a surrogate for AUC maximization.

Thanks to co-author Jadon Fowler! (second from left)



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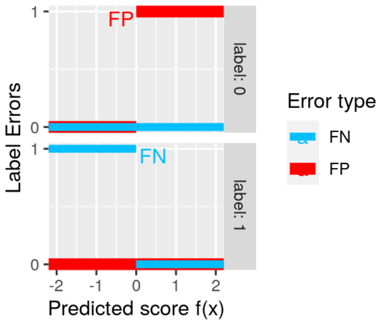
Algorithm inputs: predictions and label error functions

- Each observation $i \in \{1, \dots, n\}$ has a predicted value $\hat{y}_i \in \mathbb{R}$.
- Breakpoints $b \in \{1, \dots, B\}$ used to represent label error via tuple $(v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b)$.
- There are changes $\Delta\text{FP}_b, \Delta\text{FN}_b$ at predicted value $v_b \in \mathbb{R}$ in error function $\mathcal{I}_b \in \{1, \dots, n\}$.

Binary classification



Changepoint detection