Optimizing ROC Curves with a Sort-Based Surrogate Loss for Binary Classification and Changepoint Detection, arXiv:2107.01285

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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

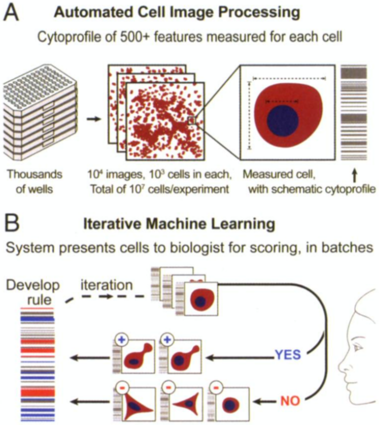
Proposed surrogate loss for ROC curve optimization: Area Under Min{FP,FN} (AUM)

Empirical results: minimizing AUM results in optimized ROC curves

Discussion and Conclusions

Problem: supervised binary classification

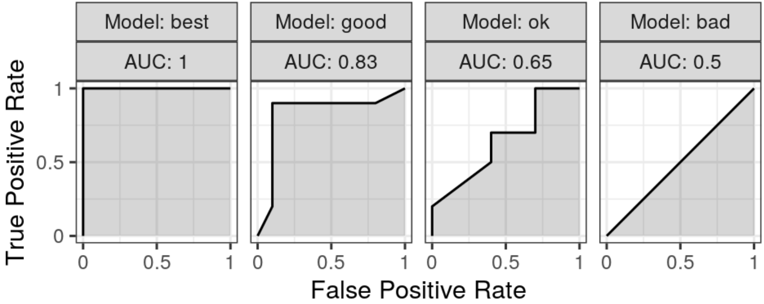
- Given pairs of inputs $\mathbf{x} \in \mathbb{R}^p$ and outputs $y \in \{0, 1\}$ can we learn a score $f(\mathbf{x}) \in \mathbb{R}$, predict $y = 1$ when $f(\mathbf{x}) > 0$?
- Example: email, $\mathbf{x}$ =bag of words, y =spam or not.
- Example: images. Jones *et al.* PNAS 2009.



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

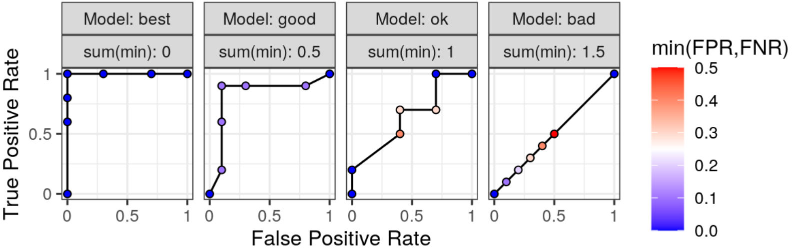
- Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- For a given set of predicted scores, plot True Positive Rate vs False Positive Rate, each point on the ROC curve is a different threshold of the predicted scores.
- Best classifier has a point near upper left (TPR=1,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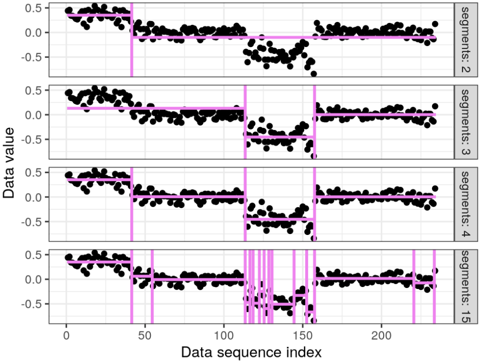
Problem: unsupervised changepoint detection

- 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)

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

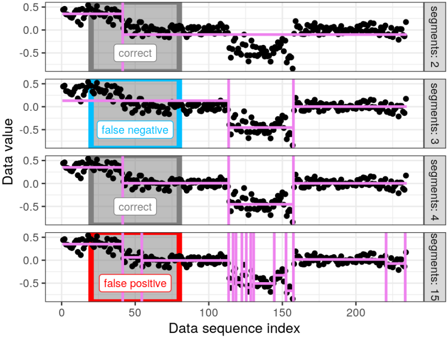


Larger penalty λ results in fewer changes/segments.

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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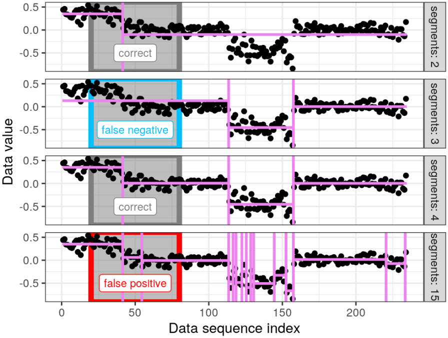
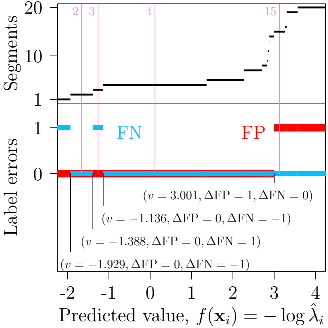
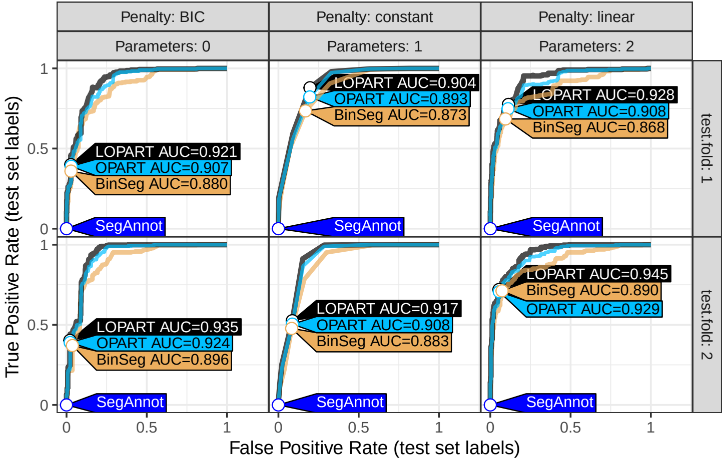




Comparing changepoint algorithms using ROC curves

Hocking TD, Srivastava A. Labeled Optimal Partitioning. Accepted in Computational Statistics, arXiv:2006.13967.



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

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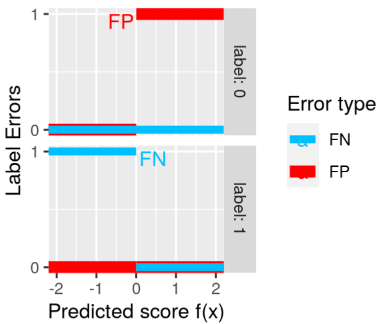
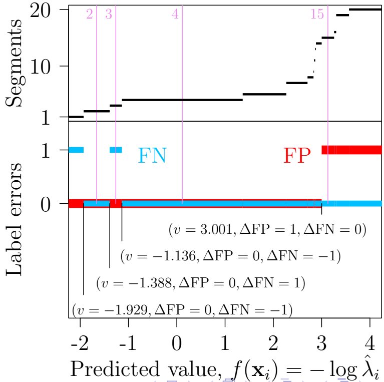
Algorithm inputs: predictions and label error functions

- Each observation $i \in \{1, \ldots, n\}$ has a predicted value $\hat{y}_i \in \mathbb{R}$.
- Breakpoints $b \in \{1, \ldots, B\}$ 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 $\mathcal{I}_b \in \{1, \ldots, n\}$.

Binary classification



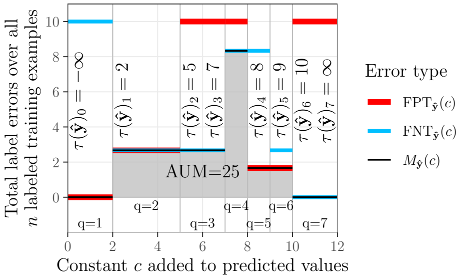
Changepoint detection

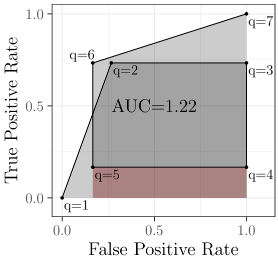


Proposed surrogate loss, Area Under Min (AUM)

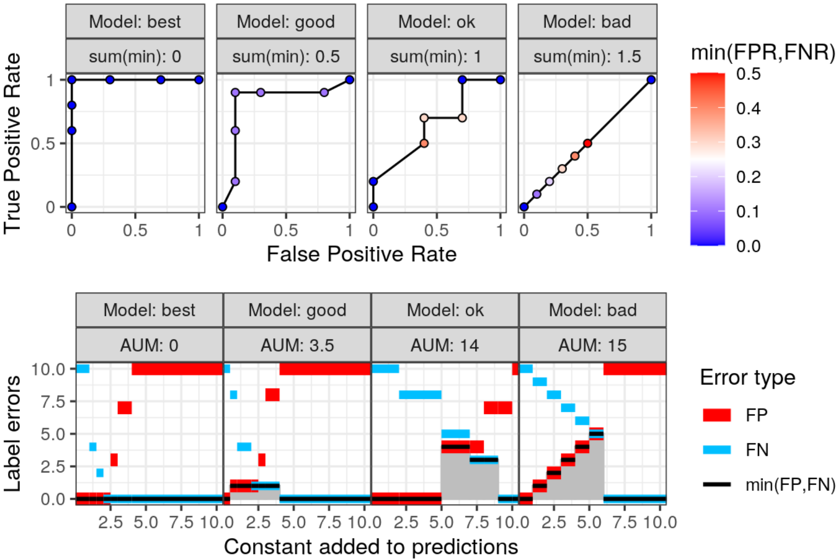
- Threshold $t_b = v_b - \hat{y}_{\mathcal{I}_b} = \tau(\hat{\mathbf{y}})_q$ is largest constant you can add to predictions and still be on ROC point q.
- Proposed surrogate loss, Area Under Min (AUM) of total FP/FN, computed via sort and modified cumsum:

$$\begin{aligned}
\underline{\text{FP}}_b &= \sum_{j: t_j < t_b} \Delta\text{FP}_j,\ \overline{\text{FP}}_b = \sum_{j: t_j \leq t_b} \Delta\text{FP}_j,\\
\underline{\text{FN}}_b &= \sum_{j: t_j \geq t_b} -\Delta\text{FN}_j,\ \overline{\text{FN}}_b = \sum_{j: t_j > t_b} -\Delta\text{FN}_j.
\end{aligned}$$





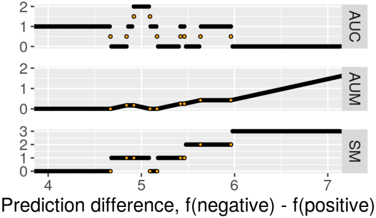
Small AUM is correlated with large AUC



Proposed algorithm computes two directional derivatives

- Gradient only defined when function is differentiable, but AUM is not differentiable everywhere (see below).
- Directional derivatives always computable (R package aum),

$$\nabla_{\mathbf{v}(-1,i)}\text{AUM}(\hat{\mathbf{y}}) =$$
$$\sum_{b:\mathcal{I}_b=i} \min\{\overline{\text{FP}}_b, \overline{\text{FN}}_b\} - \min\{\overline{\text{FP}}_b - \Delta\text{FP}_b, \overline{\text{FN}}_b - \Delta\text{FN}_b\},$$
$$\nabla_{\mathbf{v}(1,i)}\text{AUM}(\hat{\mathbf{y}}) =$$
$$\sum_{b:\mathcal{I}_b=i} \min\{\underline{\text{FP}}_b + \Delta\text{FP}_b, \underline{\text{FN}}_b + \Delta\text{FN}_b\} - \min\{\underline{\text{FP}}_b, \underline{\text{FN}}_b\}.$$



Proposed learning algo uses mean of these two directional derivatives as "gradient."

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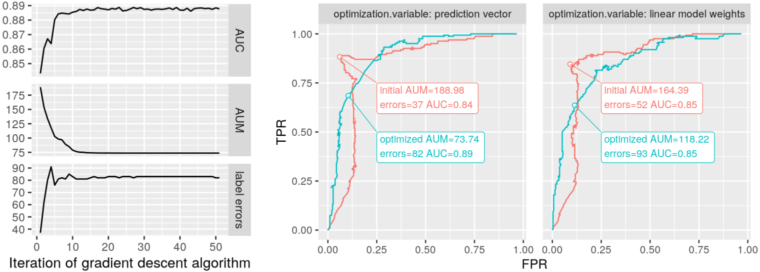
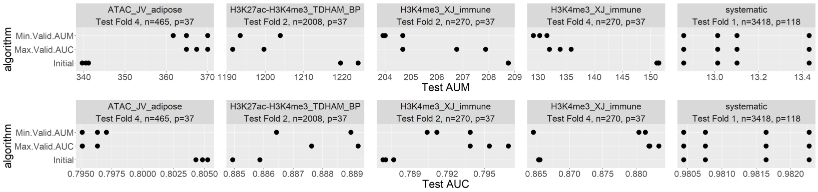
AUM gradient descent results in increased train AUC for a real changepoint problem



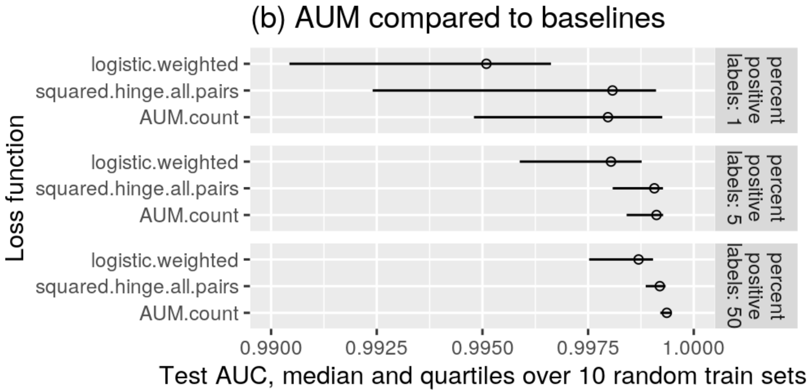
- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), gradient descent on weight vector.

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



- Five changepoint problems (panels from left to right).
- Two evaluation metrics (AUM=top, AUC=bottom).
- Three algorithms (Y axis), Initial=Min regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), Min.Valid.AUM/Max.Valid.AUC=AUM gradient descent with early stopping regularization.
- Four points = Four random initializations.

Learning algorithm competitive for unbalanced binary classification



- Squared hinge all pairs is a classic/popular surrogate loss function for AUC optimization. (Yan *et al.* ICML 2003)
- All linear models with early stopping regularization.

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Discussion and Conclusions, Pre-print arXiv:2107.01285

- ROC curves are used to evaluate binary classification and changepoint detection algorithms.
- We propose a new loss function, AUM=Area Under Min(FP,FN), which is a differentiable surrogate of the sum of Min(FP,FN) over all points on the ROC curve.
- We propose new algorithm for efficient AUM and directional derivative computation.
- Implementations available in R and python/torch: `https://cloud.r-project.org/web/packages/aum/` `https://tdhock.github.io/blog/2022/aum-learning/`
- Empirical results provide evidence that learning using AUM minimization results in ROC curve optimization (encourages monotonic/regular curves with large AUC).
- Future work: exploiting piecewise linear structure of the AUM loss, other model classes, other problems/objectives.

Thanks to co-author Jonathan Hillman! (second from left)

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