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

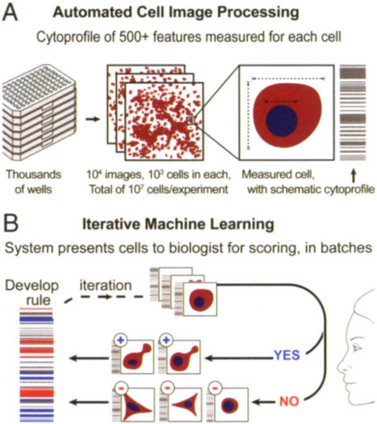
Proposed surrogate loss for ROC curve optimization: Area Under Min{FP,FN} (AUM)

Empirical results: minimizing AUM results in optimized ROC curves

Discussion and Conclusions

Problem: supervised binary classification

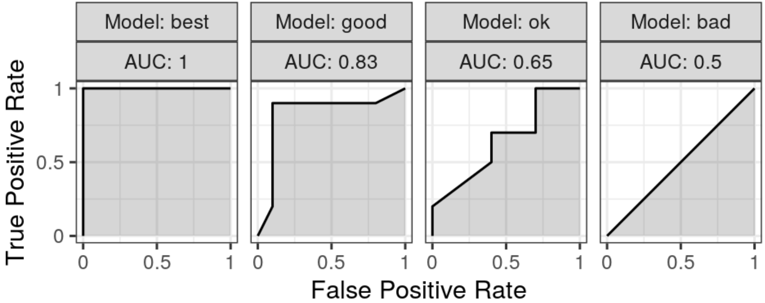
- Given pairs of inputs $\mathbf{x} \in \mathbb{R}^p$ and outputs $y \in \{0, 1\}$ can we learn a score $f(\mathbf{x}) \in \mathbb{R}$, predict $y = 1$ when $f(\mathbf{x}) > 0$?
- Example: email, $\mathbf{x}$ =bag of words, y =spam or not.
- Example: images. Jones *et al.* PNAS 2009.



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

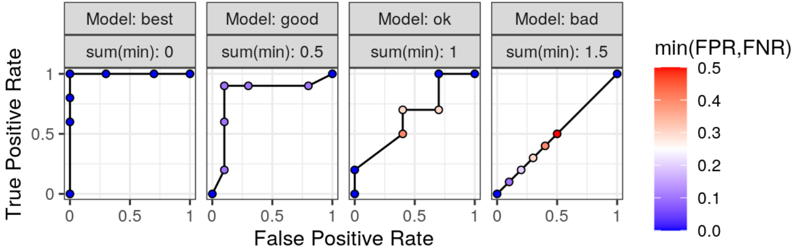
- Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- For a given set of predicted scores, plot True Positive Rate vs False Positive Rate, each point on the ROC curve is a different threshold of the predicted scores.
- Best classifier has a point near upper left (TPR=1,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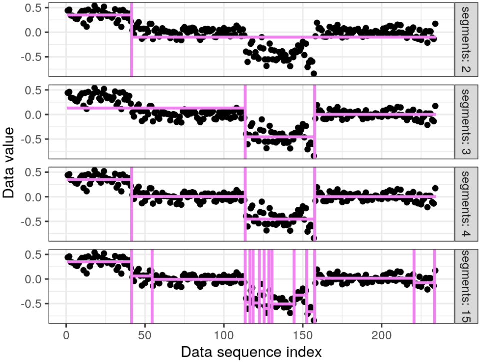
Problem: unsupervised changepoint detection

- 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)

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

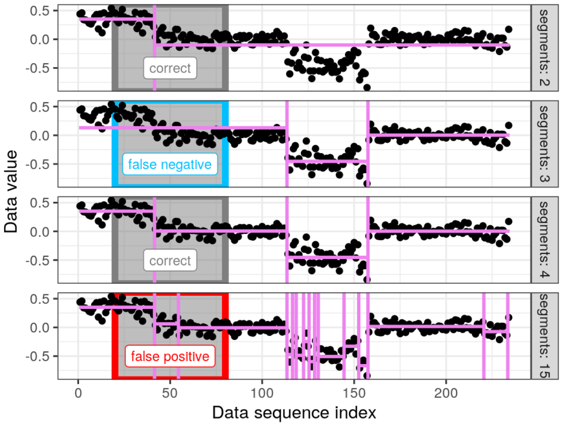


Larger penalty λ results in fewer changes/segments.

Smaller penalty λ results in more changes/segments.

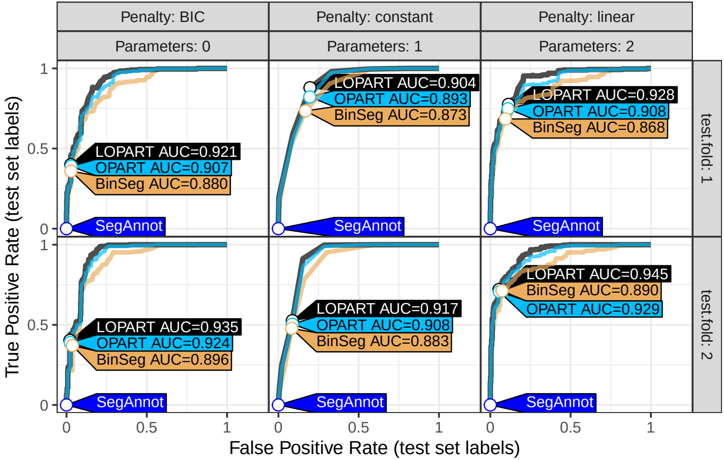
Problem: weakly supervised changepoint detection

- 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.



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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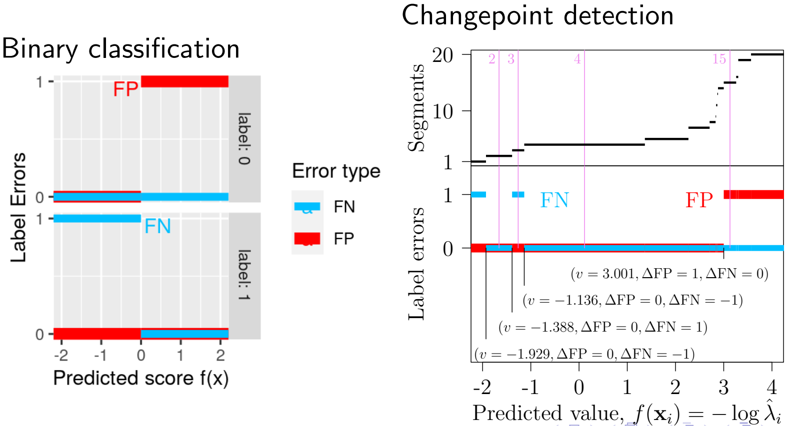
Algorithm inputs: predictions and label error functions

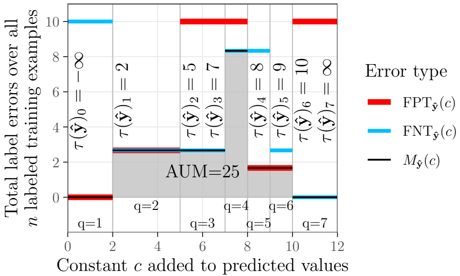
- Each observation $i \in \{1, \dots, n\}$ has a predicted value $\hat{y}_i \in \mathbb{R}$.
- Breakpoints $b \in \{1, \dots, B\}$ used to represent label error via tuple $(v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b)$.
- There are changes $\Delta\text{FP}_b, \Delta\text{FN}_b$ at predicted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

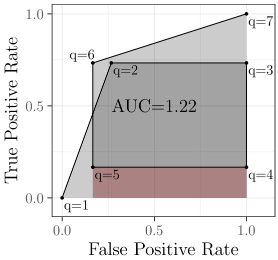


Proposed surrogate loss, Area Under Min (AUM)

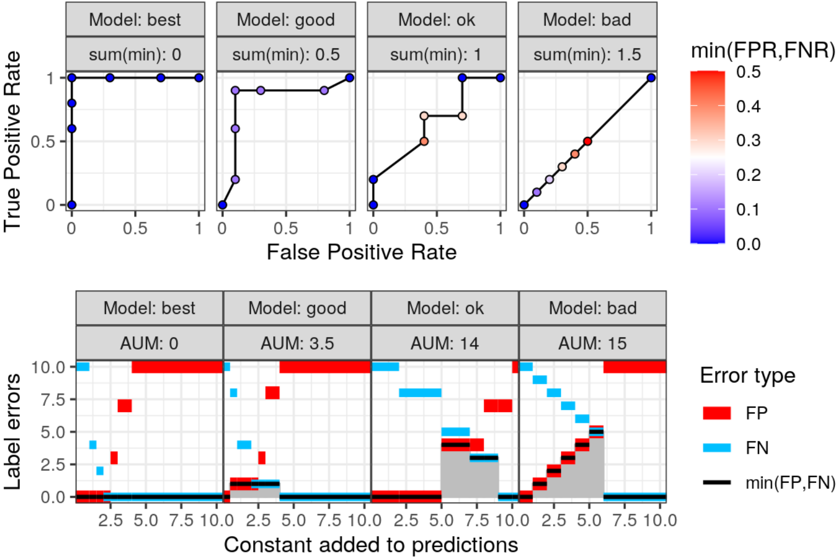
- Threshold $t_b = v_b - \hat{y}_{\mathcal{I}_b} = \tau(\hat{\mathbf{y}})_q$ is largest constant you can add to predictions and still be on ROC point q.
- Proposed surrogate loss, Area Under Min (AUM) of total FP/FN, computed via sort and modified cumsum:

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





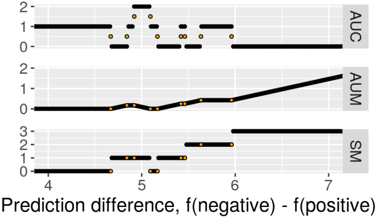
Small AUM is correlated with large AUC



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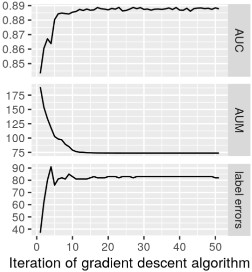
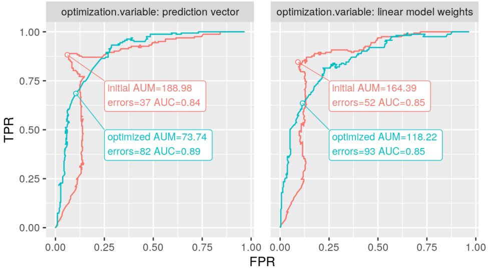
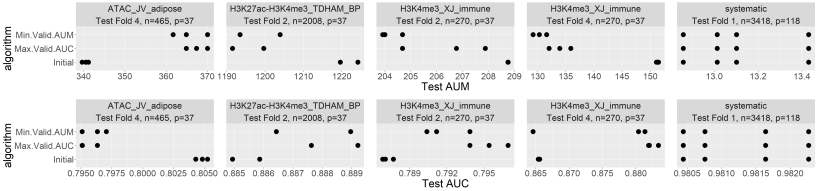
AUM gradient descent results in increased train AUC for a real changepoint problem





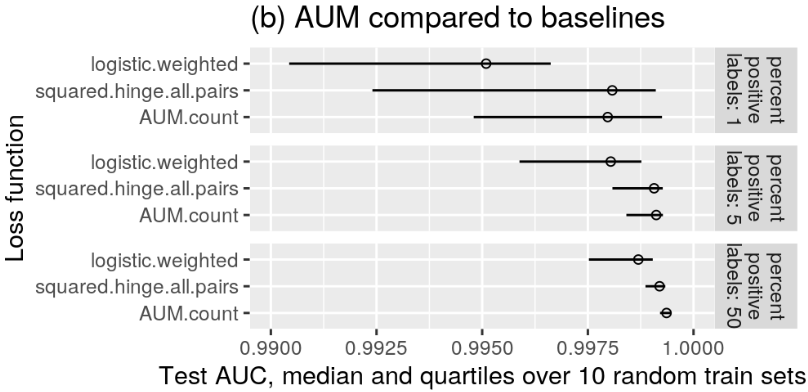
- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), gradient descent on weight vector.

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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