# Optimizing ROC Curves with a Sort-Based Surrogate Loss for Binary Classification and Changepoint Detection

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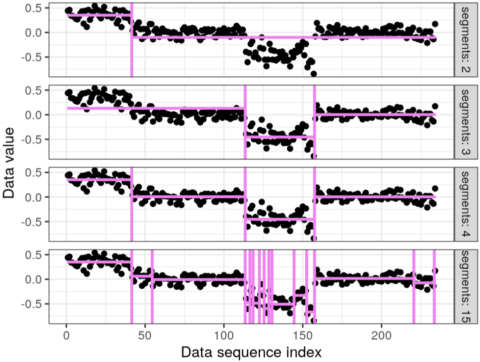
# Problem: unsupervised changepoint detection

- We are given a data sequence $z_1, \dots, z_T$ measured at $T$ points over time/space.
- Ex: DNA copy number data for cancer diagnosis, $z_t \in \mathbb{R}$.
- The penalized changepoint problem is

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

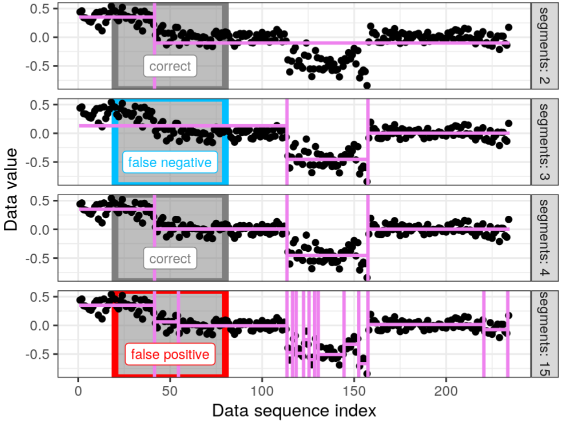



Larger penalty $\lambda$ results in fewer changes/segments.

Smaller penalty $\lambda$ results in more changes/segments.

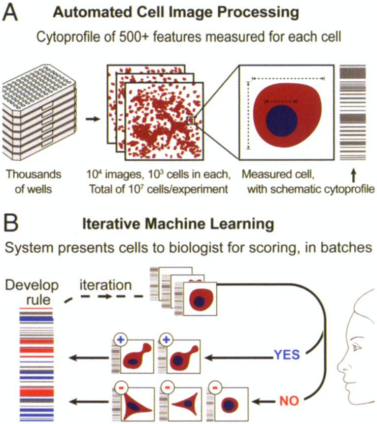
# Problem: weakly supervised changepoint detection

- 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.



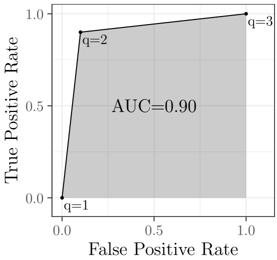
# Problem: supervised binary classification

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



# Area Under ROC curve, synthetic example

- Binary classification algo gives predictions $[\hat{y}_1, \hat{y}_2, \hat{y}_3, \hat{y}_4]$, which is one point on the ROC curve (x=FPR, y=TPR).
- Best point in ROC space is upper left (0% FPR, 100% TPR).
- Each point on the ROC curve is the FPR/TPR if you add some constant $c$ to the predictions, $[\hat{y}_1 + c, \hat{y}_2 + c, \hat{y}_3 + c, \hat{y}_4 + c]$.
- Optimizing Area Under the ROC curve (AUC) is a common objective for binary classification, especially for imbalanced data (99% positive, 1% negative labels).

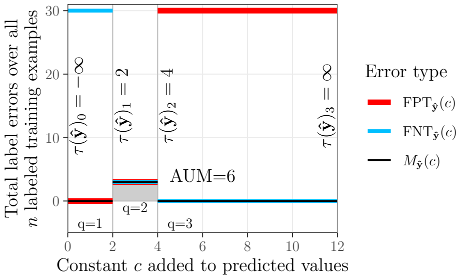


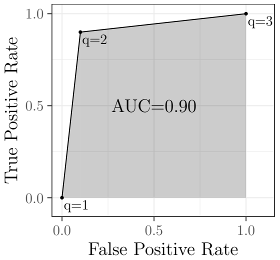

In binary classification, ROC curve is monotonic increasing.

- AUC=1 best.
- AUC=0.5 for constant prediction (usually worst).

# Area Under ROC curve, synthetic example

- Example: label = [-1, -1, 1, 1], predictions [-8, -5, -5, -8], No constant added $c = 0$, $q = 1$ in this example (everything predicted negative, so no false positives, but no true positives).
- Add $c = 6 \Rightarrow$ [-2, 1, 1, -2], some FP and TP, $q = 2$
- Add $c = 9 \Rightarrow$ [7, 4, 4, 7], all FP and TP, $q = 3$.

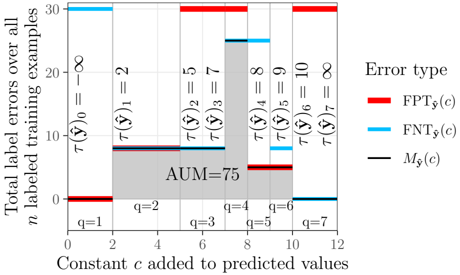


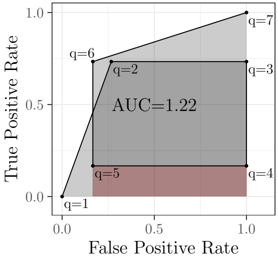



# Looping ROC curve, simple synthetic example

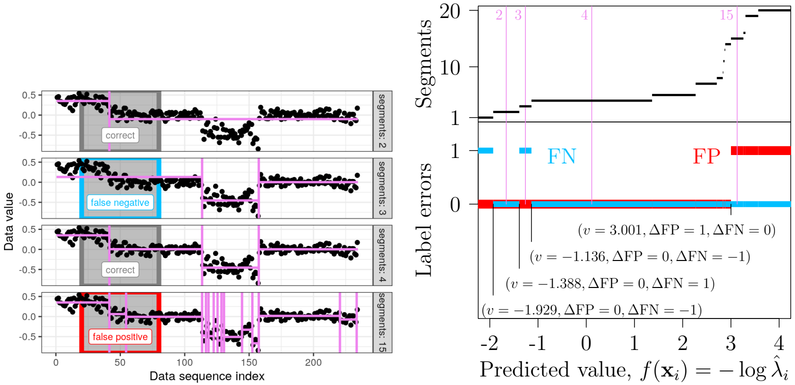
If ROC curve has loops, AUC can be greater than one.

- Dark grey area double counted.
- Red area negative counted.
- Do we want to maximize AUC?
- Minimize Area Under Min (AUM) instead, which pushes ROC points toward upper left.



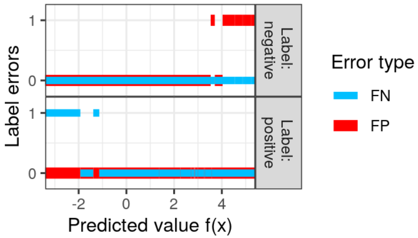



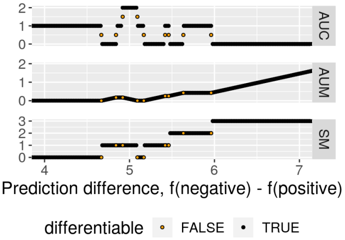
# Real data example with non-monotonic label error




Optimal changepoint model may have non-monotonic error (for example FN), because changepoints at model size $s$ may not be present in model $s + 1$.

# Real data example with AUC greater than one




- $n = 2$ labeled changepoint problems.
- AUC=2 when prediction difference=5.
- AUM=0 implies AUC=1.
- AUM is convex relaxation of non-convex Sum of Min (SM).
- AUM is differentiable almost everywhere; compute the gradient and use it for learning.

## Definition of data set, notations

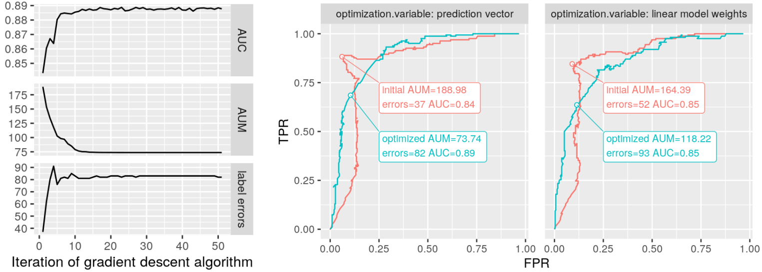
- Let there be a total of $B$ breakpoints in the error functions over all $n$ labeled training examples.
- Each breakpoint $b \in \{1, \dots, B\}$ is represented by the tuple $(v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b)$, where the $\mathcal{I}_b \in \{1, \dots, n\}$ is an example index, and there are changes $\Delta\text{FP}_b, \Delta\text{FN}_b$ at predicted value $v_b \in \mathbb{R}$ in the error functions.
- For example in binary classification, there are $B = n$ breakpoints (same as the number of labeled training examples); for each breakpoint $b \in \{1, \dots, B\}$ we have $v_b = 0$ and $\mathcal{I}_b = b$. For breakpoints $b$ with positive labels $y_b = 1$ we have $\Delta\text{FP} = 0, \Delta\text{FN} = -1$, and for negative labels $y_b = -1$ we have $\Delta\text{FP} = 1, \Delta\text{FN} = 0$.
- In changepoint detection we have more general error functions, which may have more than one breakpoint per example.

# Proposed algorithm uses sort to compute AUM and directional derivatives

- Gradient only defined when function is differentiable, but AUM is not everywhere.
- Directional derivatives defined everywhere.
- Overall $O(B \log B)$ time due to sort.

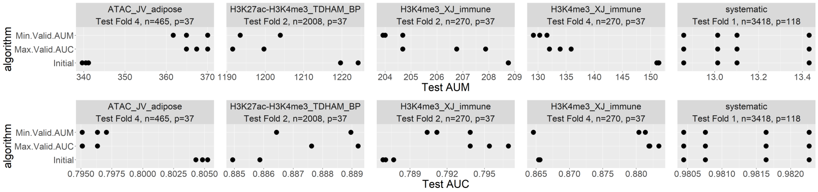
**Input:** Predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$, breakpoints in error functions $v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b$ for all $b \in \{1, \dots, B\}$.
Zero the AUM $\in \mathbb{R}$ and directional derivatives $\mathbf{D} \in \mathbb{R}^{n \times 2}$.
$t_b \leftarrow v_b - \hat{y}_{\mathcal{I}_b}$ for all $b$.
$s_1, \dots, s_B \leftarrow \textsc{SortedIndices}(t_1, \dots, t_B)$.
Compute $\underline{\text{FP}}_b, \overline{\text{FP}}_b, \underline{\text{FN}}_b, \overline{\text{FN}}_b$ for all $b$ using $s_1, \dots, s_B$.
**for** $b \in \{2, \dots, B\}$ **do**
    AUM $\mathrel{+}= (t_{s_b} - t_{s_{b-1}}) \min\{\underline{\text{FP}}_b, \overline{\text{FN}}_b\}$.
**for** $b \in \{1, \dots, B\}$ **do**
    $\mathbf{D}_{\mathcal{I}_b,1} \mathrel{+}= \min\{\overline{\text{FP}}_b, \overline{\text{FN}}_b\} - \min\{\overline{\text{FP}}_b - \Delta\text{FP}_b, \overline{\text{FN}}_b - \Delta\text{FN}_b\}$
    $\mathbf{D}_{\mathcal{I}_b,2} \mathrel{+}= \min\{\underline{\text{FP}}_b + \Delta\text{FP}_b, \underline{\text{FN}}_b + \Delta\text{FN}_b\} - \min\{\underline{\text{FP}}_b, \underline{\text{FN}}_b\}$
**Output:** AUM and matrix $\mathbf{D}$ of directional derivatives.

# Train set ROC curves for a real changepoint problem



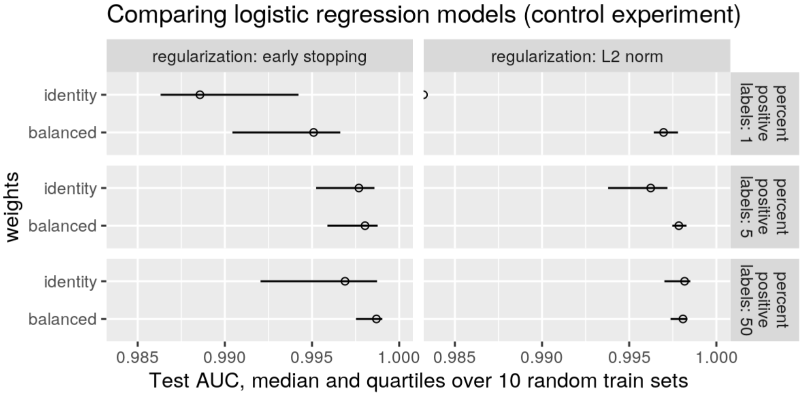

- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error), gradient descent on weight vector.

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



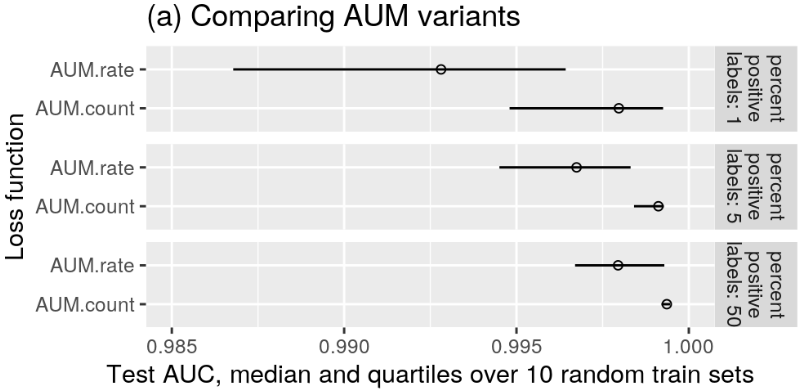

- Five changepoint problems (panels from left to right).
- Two evaluation metrics (AUM=top, AUC=bottom).
- Three algorithms (Y axis), Initial=Min regularized convex loss (surrogate for label error), Min.Valid.AUM/Min.Valid.AUC=AUM gradient descent with early stopping regularization.

# Standard logistic loss fails for highly imbalanced labels



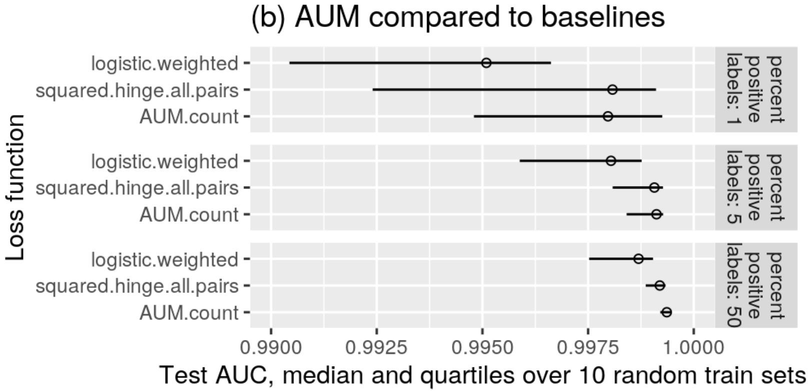

- Test set has 50% positive, 50% negative labels.
- Train set has variable class imbalance (panels top to bottom).
- Loss is $\ell[f(x_i), y_i]w_i$ with $w_i = 1$ for identity weights, $w_i = 1/N_{y_i}$ for balanced, ex: 1% position means $w_i \in \{1/10, 1/990\}$.

# Error rate loss is not as useful as error count loss



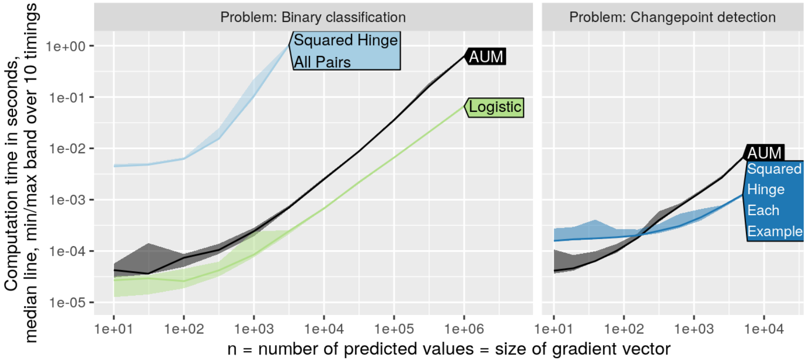

- AUM.count is as described previously: error functions used to compute Min(FP,FN) are absolute label counts.
- AUM.rate is a variant which uses normalized error functions, Min(FPR,FNR).
- Both linear models with early stopping regularization.

# Learning algorithm competitive for unbalanced binary classification




- Squared hinge all pairs is a classic/popular surrogate loss function for AUC optimization.
- All linear models with early stopping regularization.

# Comparable computation time to other loss functions




- Logistic $O(n)$.
- AUM $O(n \log n)$.
- Squared Hinge All Pairs $O(n^2)$.
- Squared Hinge Each Example $O(n)$.

# Conclusions, Pre-print arXiv:2107.01285

- ROC curves are used to evaluate binary classification and changepoint detection algorithms.
- In changepoint detection there can be loops in ROC curves, so maximizing AUC may not be desirable.
- Instead we propose to minimize a new loss, AUM=Area Under Min(FP,FN).
- We propose new algorithm for efficient AUM and directional derivative computation.
- Empirical results provide evidence that learning using AUM minimization results in AUC maximization.
- Future work: sort-based surrogates for all pairs loss functions (binary classification, information retreival).

# Thanks!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# More notation

First let $\{(\text{fpt}(\hat{\mathbf{y}})_q, \text{fnt}(\hat{\mathbf{y}})_q, \tau(\hat{\mathbf{y}})_q)\}_{q=1}^Q$ be a sequence of $Q$ tuples, each of which corresponds to a point on the ROC curve (Figure **??**, right). The fpt/fnt are false positive/negative totals whereas $\tau$ are values such there is a change/threshold at $M_{\hat{\mathbf{y}}}(\tau)$. As shown in Figure **??** we assume these values are increasing, $-\infty = \tau(\hat{\mathbf{y}})_0 < \cdots < \tau(\hat{\mathbf{y}})_Q = \infty$. For each $q \in \{1, \ldots, Q\}$ there is a corresponding interval of values $c$ between $\tau(\hat{\mathbf{y}})_{q-1}$ and $\tau(\hat{\mathbf{y}})_q$ such that $\text{FPT}_{\hat{\mathbf{y}}}(c) = \text{fpt}(\hat{\mathbf{y}})_q$ and $\text{FNT}_{\hat{\mathbf{y}}}(c) = \text{fnt}(\hat{\mathbf{y}})_q$ for all $c \in (\tau(\hat{\mathbf{y}})_{q-1}, \tau(\hat{\mathbf{y}})_q)$ (Figure **??**, left). Then we define $m(\hat{\mathbf{y}})_q = \min\{\text{fpt}(\hat{\mathbf{y}})_q, \text{fnt}(\hat{\mathbf{y}})_q\}$ and so since $m(\hat{\mathbf{y}})_1 = m(\hat{\mathbf{y}})_Q = 0$ the area under those intervals is zero, and the AUM can be computed by summing over all of the other intervals,

# L1 relaxation interpretation

Our proposed loss function is

$$\text{AUM}(\hat{\mathbf{y}}) = \sum_{q=2}^{Q-1} [\tau(\hat{\mathbf{y}})_q - \tau(\hat{\mathbf{y}})_{q-1}] m(\hat{\mathbf{y}})_q.$$

It is an L1 relaxation of the following non-convex **S**um of **M**in(FP,FN) function,

$$\text{SM}(\hat{\mathbf{y}}) = \sum_{q=2}^{Q-1} I[\tau(\hat{\mathbf{y}})_q \neq \tau(\hat{\mathbf{y}})_{q-1}] m(\hat{\mathbf{y}})_q = \sum_{q:\tau(\hat{\mathbf{y}})_q \neq \tau(\hat{\mathbf{y}})_{q-1}} m(\hat{\mathbf{y}})_q.$$

# FP and FN counts before/after each threshold

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

# Directional derivatives

**Theorem**

*The AUM directional derivatives for a particular example $i \in \{1, \dots, n\}$ can be computed using the following equations.*

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

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