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

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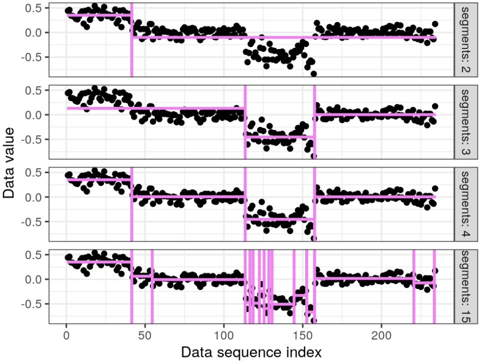
Problem: unsupervised changepoint detection

- 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

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

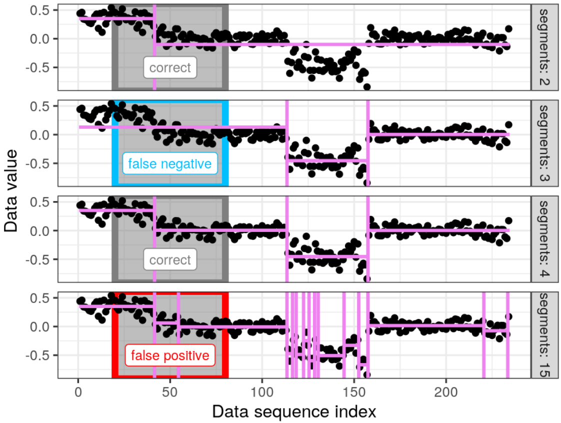


Larger penalty λ results in fewer changes/segments.

Smaller penalty λ results in more changes/segments.

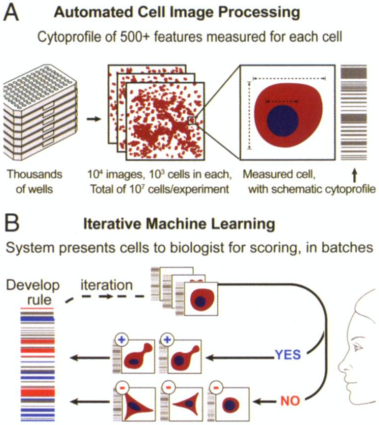
Problem: weakly supervised changepoint detection

- 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.



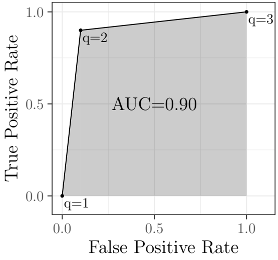
Problem: supervised binary classification

- 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.



Receiver Operating Characteristic (ROC) curve

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

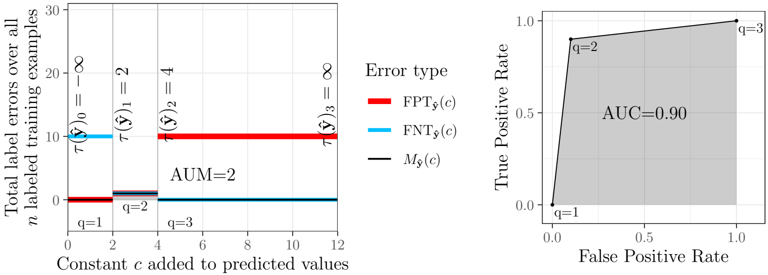


In binary classification, ROC curve is monotonic increasing.

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

Area Under ROC curve, synthetic example

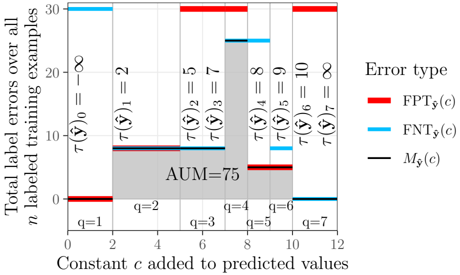
- label = [1,0,0,...,1,1,0] (20 labels, 10 positive, 10 negative).
- predictions = [-4, -4, -4, ..., -2, -2, -2].
- No constant added $c = 0$, $q = 1$, everything predicted negative, so no false positives, but no true positives.
- Add $c = 3 \Rightarrow$ [-1, -1, -1, ..., 1, 1, 1], 1 FP and 9 TP, $q = 2$.
- Add $c = 5 \Rightarrow$ [1, 1, 1, ..., 3, 3, 3], all FP and TP, $q = 3$.

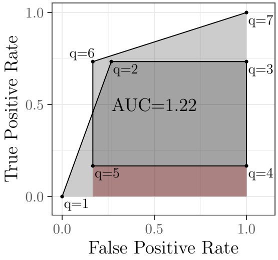


Looping ROC curve, simple synthetic example

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

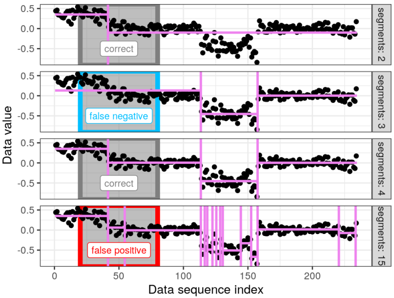
- Dark grey area double counted.
- Red area negative counted.
- Do we want to maximize AUC?
- Minimize Area Under Min (AUM) instead, which encourages ROC points in upper left.

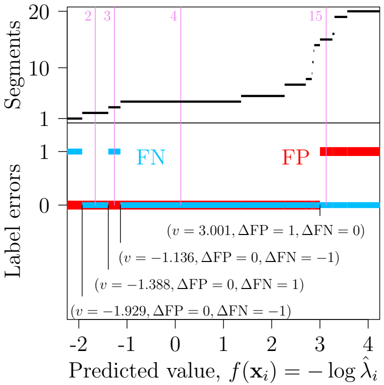




Real data example with non-monotonic label error

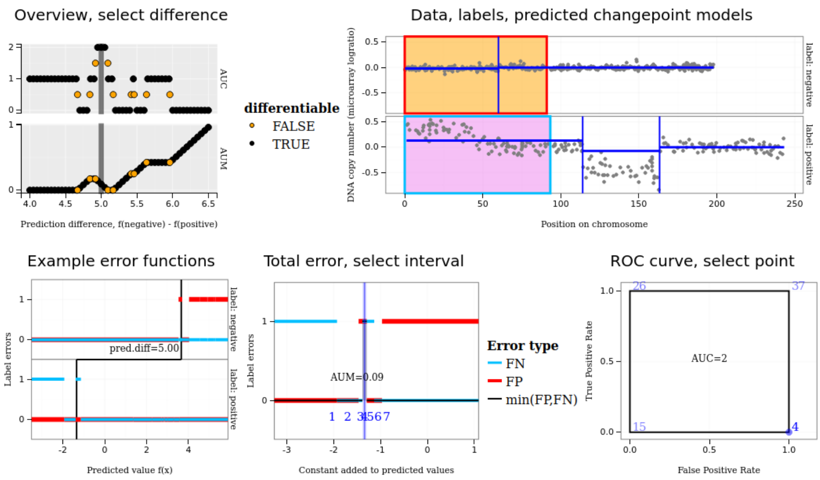
ROC curve loops result from non-monotonic FP/FN functions, but do these occur in real data? Yes, in supervised changepoint problems.





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, interactive AUC/AUM demo



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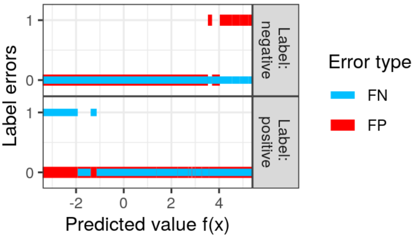
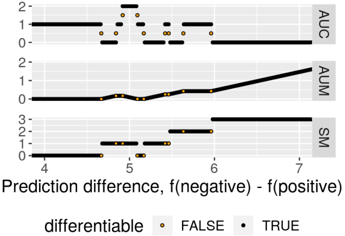
Real data example with AUC greater than one

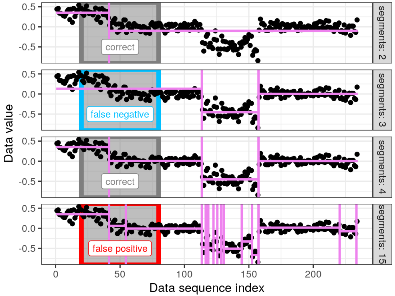


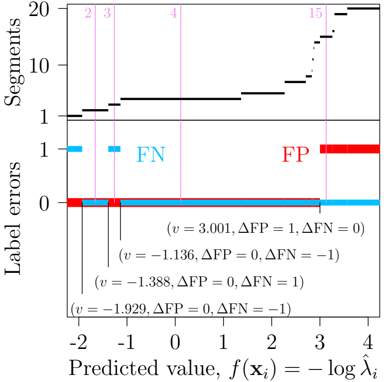


- $n = 2$ labeled changepoint problems.
- AUC=2 when prediction difference=5.
- AUM=0 implies AUC=1.
- AUM is convex relaxation of non-convex Sum of Min (SM).
- AUM is differentiable almost everywhere.
- Main new idea: compute the gradient of this function and use it for learning.

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 $\mathcal{I}_b \in \{1, \ldots, n\}$.



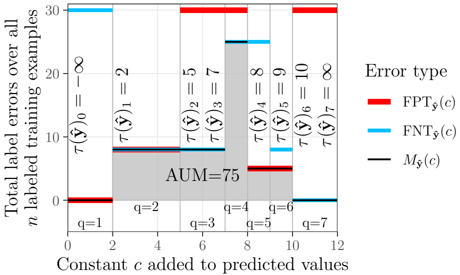


Algorithm computes total FP and FN for each threshold/constant added to predicted values

- Breakpoint threshold, $t_b = v_b - \hat{y}_{\mathcal{I}_b} = \tau(\hat{\mathbf{y}})_q$ for some q.
- Total error before/after each breakpoint can be computed via sort and modified cumsum:

$$\underline{\mathrm{FP}}_b = \sum_{j:t_j<t_b} \Delta \mathrm{FP}_j,\ \overline{\mathrm{FP}}_b = \sum_{j:t_j\leq t_b} \Delta \mathrm{FP}_j,$$

$$\underline{\mathrm{FN}}_b = \sum_{j:t_j\geq t_b} -\Delta \mathrm{FN}_j,\ \overline{\mathrm{FN}}_b = \sum_{j:t_j>t_b} -\Delta \mathrm{FN}_j.$$



Algorithm computes two directional derivatives

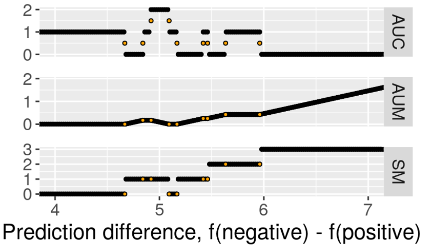
- Gradient only defined when function is differentiable, but AUM is not everywhere (see below).
- Directional derivatives defined everywhere.

$$\nabla_{\mathbf{v}(-1,i)}\text{AUM}(\hat{\mathbf{y}}) =$$

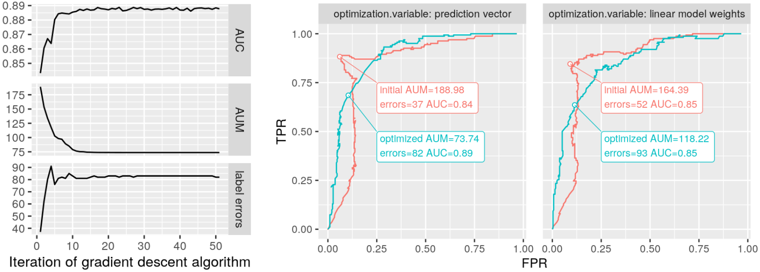
$$\sum_{b:\mathcal{I}_b=i} \min\{\overline{\text{FP}}_b, \overline{\text{FN}}_b\} - \min\{\overline{\text{FP}}_b - \Delta\text{FP}_b, \overline{\text{FN}}_b - \Delta\text{FN}_b\},$$

$$\nabla_{\mathbf{v}(1,i)}\text{AUM}(\hat{\mathbf{y}}) =$$

$$\sum_{b:\mathcal{I}_b=i} \min\{\underline{\text{FP}}_b + \Delta\text{FP}_b, \underline{\text{FN}}_b + \Delta\text{FN}_b\} - \min\{\underline{\text{FP}}_b, \underline{\text{FN}}_b\}.$$

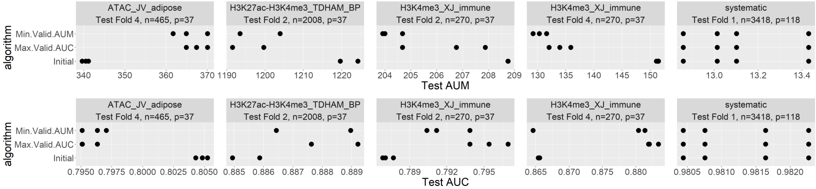


Train set ROC curves for a real changepoint problem



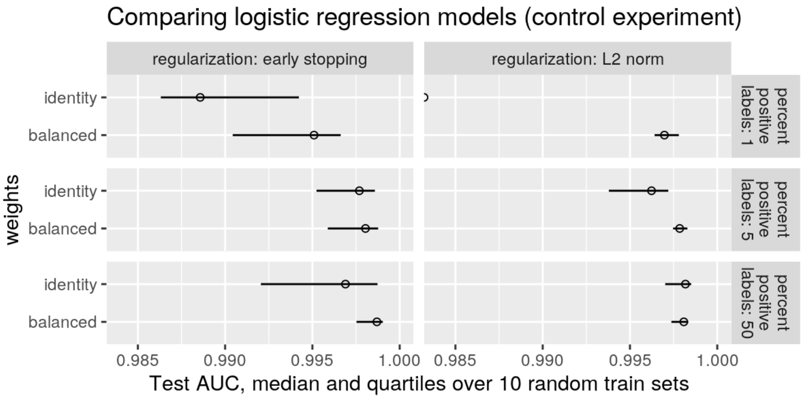
- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error), gradient descent on weight vector.

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



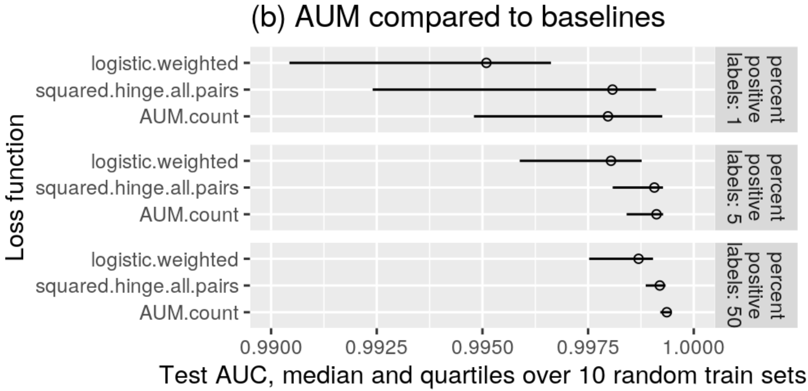
- Five changepoint problems (panels from left to right).
- Two evaluation metrics (AUM=top, AUC=bottom).
- Three algorithms (Y axis), Initial=Min regularized convex loss (surrogate for label error), Min.Valid.AUM/Min.Valid.AUC=AUM gradient descent with early stopping regularization.

Standard logistic loss fails for highly imbalanced labels



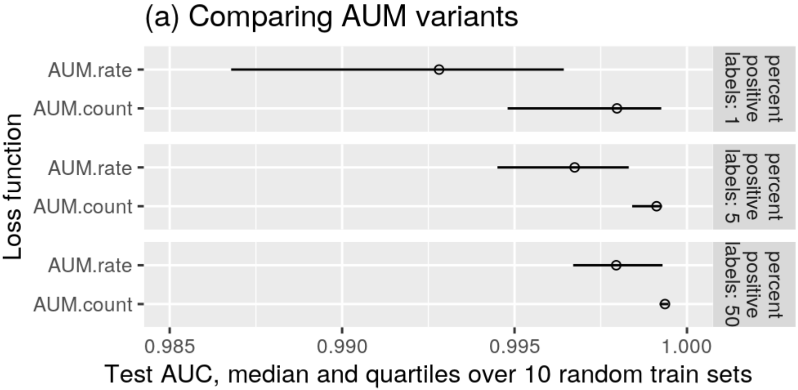
- Test set has 50% positive, 50% negative labels.
- Train set has variable class imbalance (panels top to bottom).
- Loss is $\ell[f(x_i), y_i]w_i$ with $w_i = 1$ for identity weights, $w_i = 1/N_{y_i}$ for balanced, ex: 1% position means $w_i \in \{1/10, 1/990\}$.

Learning algorithm competitive for unbalanced binary classification



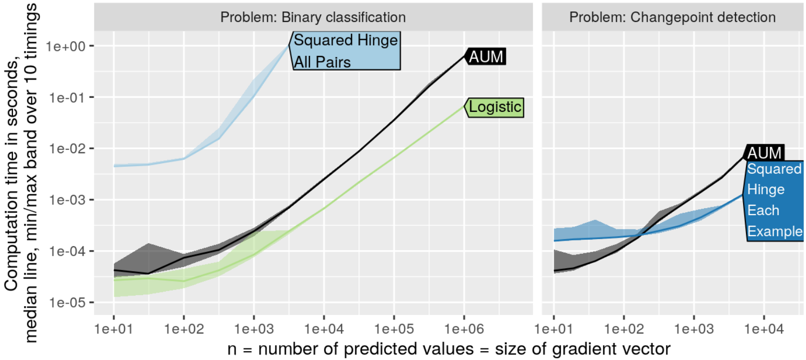
- Squared hinge all pairs is a classic/popular surrogate loss function for AUC optimization.
- All linear models with early stopping regularization.

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.

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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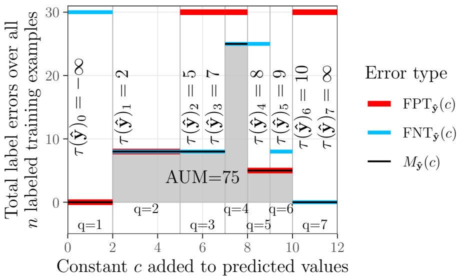
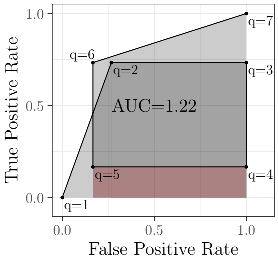
More notation

- 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 (and an interval on the fn/fp error plot).
- For each q the $\text{fpt}(\hat{\mathbf{y}})_q, \text{fpt}(\hat{\mathbf{y}})_q$ are false positive/negative totals at that point (in that interval) whereas $\tau(\hat{\mathbf{y}})_q$ is the upper limit of the interval.
- The limits are increasing, $-\infty = \tau(\hat{\mathbf{y}})_0 < \cdots < \tau(\hat{\mathbf{y}})_Q = \infty$.
- Then we define $m(\hat{\mathbf{y}})_q = \min\{\text{fpt}(\hat{\mathbf{y}})_q, \text{fnt}(\hat{\mathbf{y}})_q\}$ as the min of fp and fn totals in that interval.





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,

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

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

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 $+= (t_{s_b} - t_{s_{b-1}}) \min\{\underline{\text{FP}}_b, \overline{\text{FN}}_b\}$.

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.

- Overall $O(B \log B)$ time due to sort.