

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

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Problem Setting and Related Work

Proposed algorithm

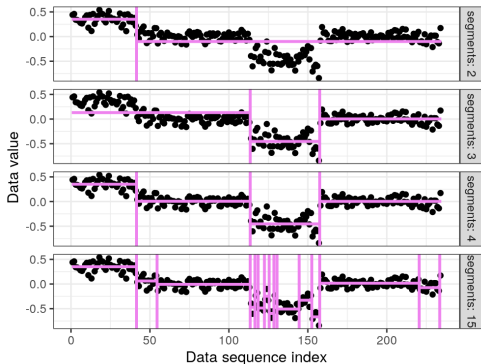
Empirical results

Discussion and Conclusions

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)

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

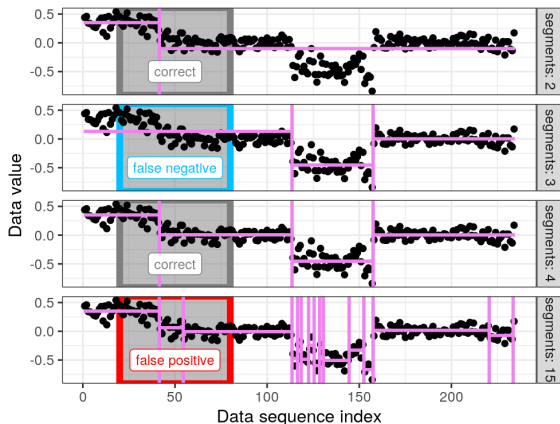


Larger penalty λ
results in fewer
changes/segments.

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.

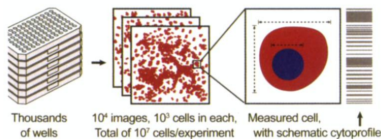


Problem: supervised binary classification

- ▶ 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.

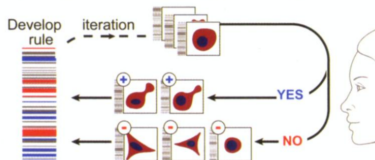
A Automated Cell Image Processing

Cytoprofile of 500+ features measured for each cell



B Iterative Machine Learning

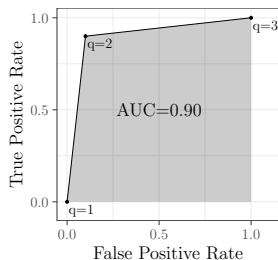
System presents cells to biologist for scoring, in batches



Receiver Operating Characteristic (ROC) curve

Classic evaluation method from the signal processing literature (Egan and Egan, 1975).

- ▶ 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 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).

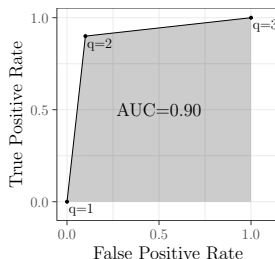
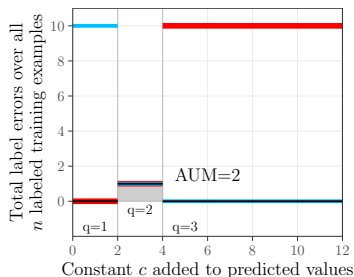


In binary classification, ROC curve is monotonic increasing.

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

Area Under ROC curve, synthetic example

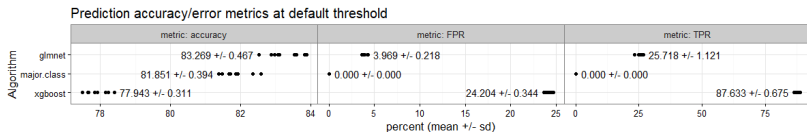
- ▶ Labels = $[1, 0, 0, \dots, 1, 1, 0]$ (20 labels, 10 positive, 10 negative).
- ▶ Predictions = $[-4, -4, -4, \dots, -2, -2, -2]$.
- ▶ No constant added $c = 0$, $q = 1$, everything predicted negative, so no false positives, but no true positives.
- ▶ Add $c = 3 \Rightarrow [-1, -1, -1, \dots, 1, 1,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



Real data example when ROC curves are useful

Data from collaboration with SICCS professor Patrick Jantz, about predicting presence/absence of trees in different locations.

- ▶ glmnet: L1-regularized linear model.
- ▶ major.class: featureless baseline (ignores inputs, always predicts most frequent class label in train set)
- ▶ xgboost: gradient boosted decision trees.
- ▶ Which algorithm is the most accurate?



<https://bl.ocks.org/tdhock/raw/172d0f68a51a8de5d6f1bed7f23f5f82/>

Problem Setting and Related Work

Proposed algorithm

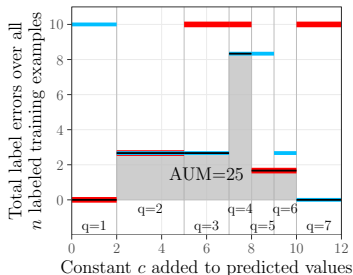
Empirical results

Discussion and Conclusions

Looping ROC curve, simple synthetic example

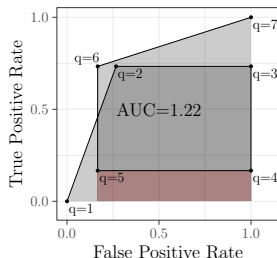
If ROC curve has loops, AUC can be greater than one, but with some very sub-optimal points (large min error, for example $q=4$).

- ▶ Dark grey area double counted.
- ▶ Red area negative counted.
- ▶ Do we want to maximize AUC?
- ▶ Minimize Area Under Min (AUM) instead, which encourages monotonic ROC curve with points in upper left (small min error, for example $q=1,6,7$).



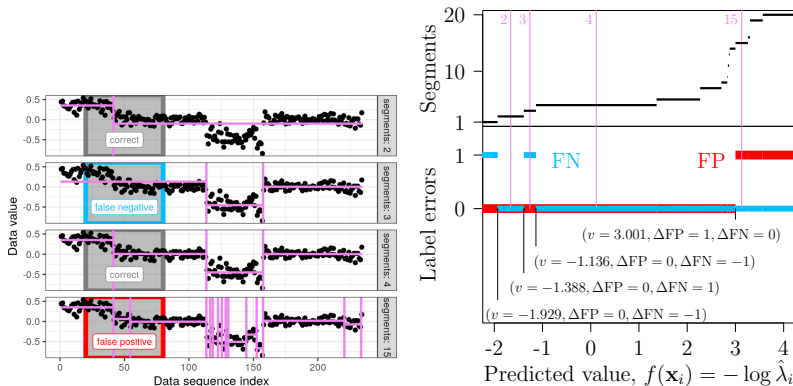
Error type

- $FPT_{\hat{y}}(c)$
- $FNT_{\hat{y}}(c)$
- $M_{\hat{y}}(c)$



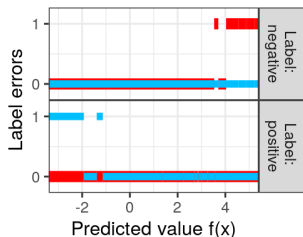
Real data example with non-monotonic label error

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 $s + 1$.

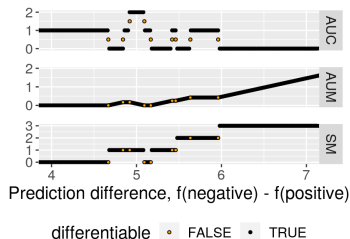
Real data example with AUC greater than one



Error type

FN

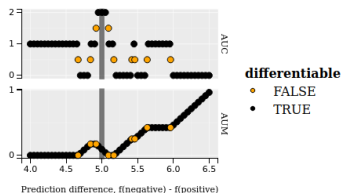
FP



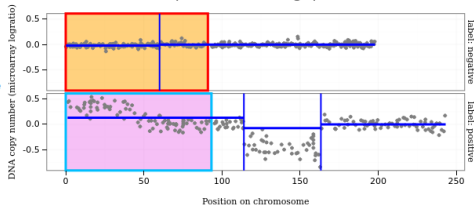
- ▶ $n = 2$ labeled changepoint problems.
- ▶ $\text{AUC} = 2$ when prediction difference = 5.
- ▶ $\text{AUM} = 0$ implies $\text{AUC} = 1$.
- ▶ AUM is convex relaxation of non-convex Sum of Min (SM).
- ▶ AUM is differentiable almost everywhere.
- ▶ Main new idea: compute the gradient of this function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

Real data example, interactive AUC/AUM demo

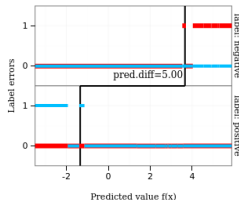
Overview, select difference



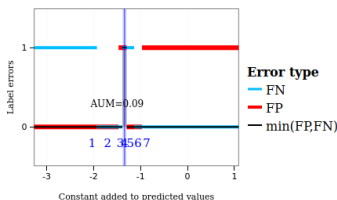
Data, labels, predicted changepoint models



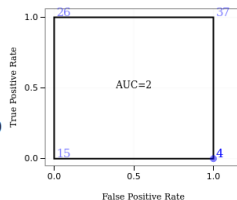
Example error functions



Total error, select interval



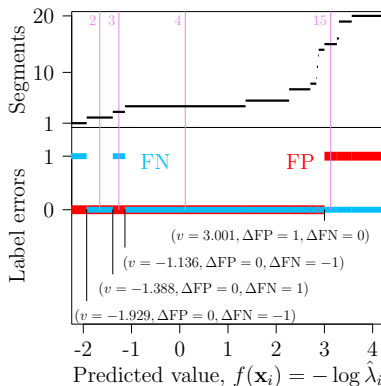
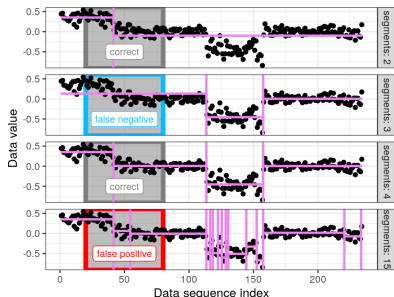
ROC curve, select point



<http://bl.ocks.org/tdhock/raw/e3f56fa419a6638f943884a3abe1dc0b/>

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 $(v_b, \Delta FP_b, \Delta FN_b, \mathcal{I}_b)$.
- ▶ There are changes $\Delta FP_b, \Delta FN_b$ at predicted value $v_b \in \mathbb{R}$ in error function $\mathcal{I}_b \in \{1, \dots, n\}$.

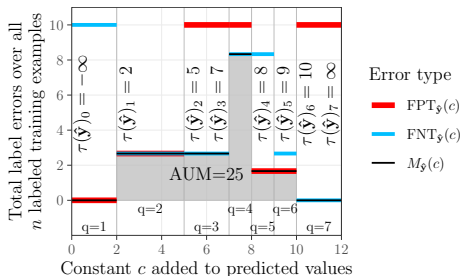


Algorithm computes total FP and FN for each threshold/constant added to predicted values

- ▶ 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:

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

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



Algorithm computes two directional derivatives

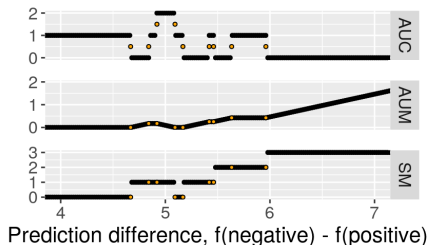
- ▶ Gradient only defined when function is differentiable, but AUM is not differentiable everywhere (see below).
- ▶ Directional derivatives defined everywhere.

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

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

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

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



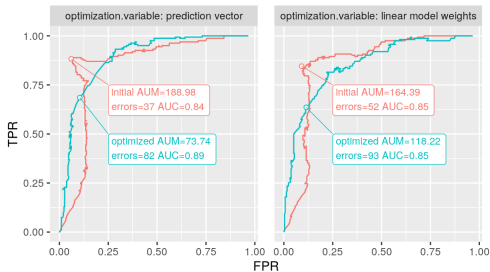
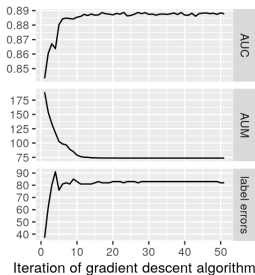
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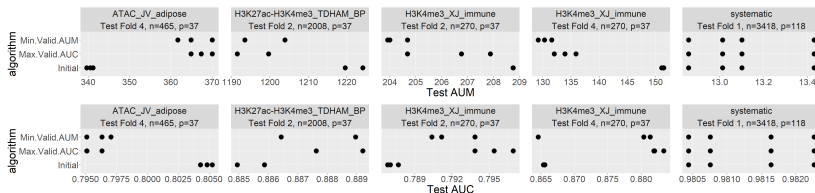
Discussion and Conclusions

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.

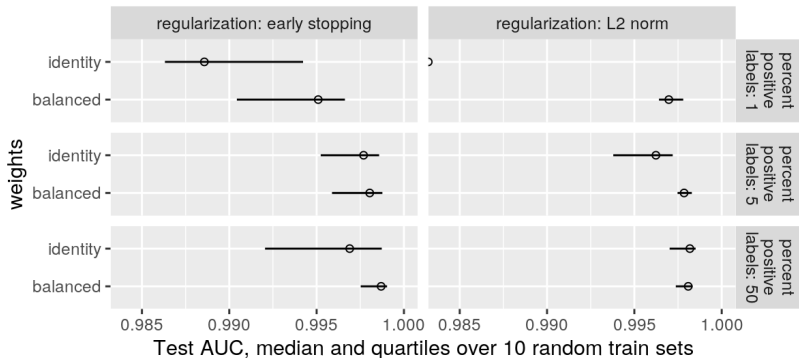
Learning algorithm results in better test AUC/AUM for changepoint problems



- ▶ 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.

Standard logistic loss fails for highly imbalanced labels

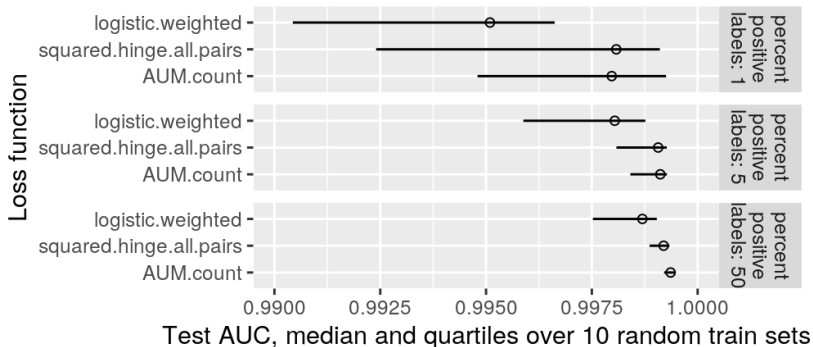
Comparing logistic regression models (control experiment)



- ▶ Subset of zip.train/zip.test data (only 0/1 labels).
- ▶ Test set size 528 with balanced labels (50%/50%).
- ▶ Train set size 1000 with variable class imbalance.
- ▶ 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% positive means $w_i \in \{1/10, 1/990\}$.

Learning algorithm competitive for unbalanced binary classification

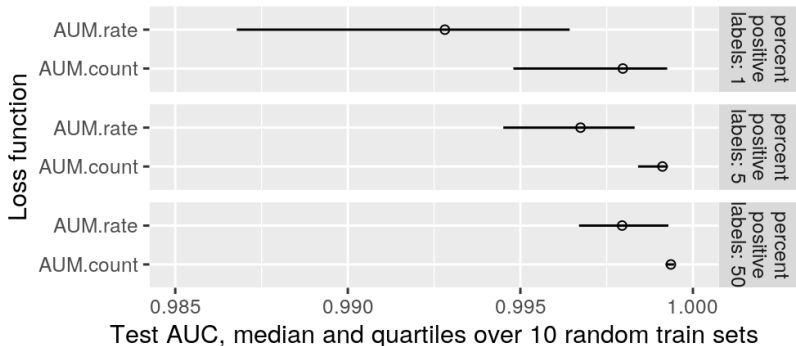
(b) AUM compared to baselines



- ▶ 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.

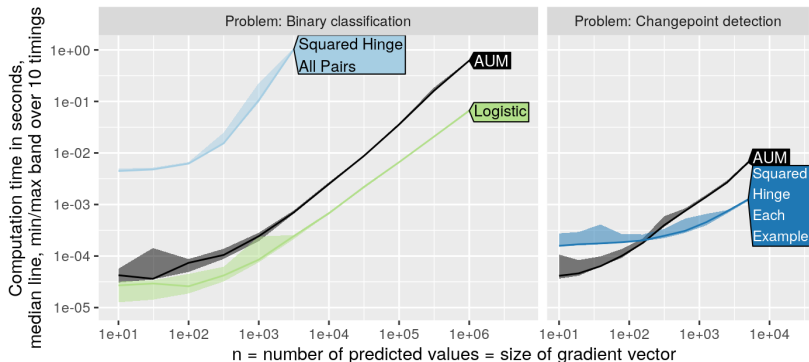
Error rate loss is not as useful as error count loss

(a) Comparing AUM variants



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

Comparable computation time to other loss functions



- ▶ Logistic $O(n)$.
- ▶ AUM $O(n \log n)$. (proposed)
- ▶ Squared Hinge All Pairs $O(n^2)$. (Yan *et al.* ICML 2003)
- ▶ Squared Hinge Each Example $O(n)$. (Hocking *et al.* ICML 2013)

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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, $AUM = \text{Area Under Min}(FP, FN)$.
- ▶ 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 retrieval).

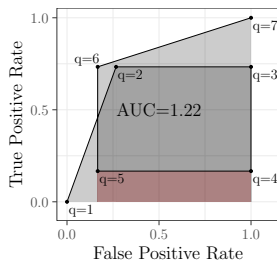
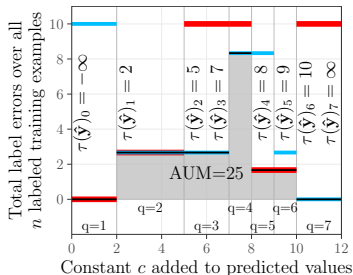
Thanks to co-author Jonathan Hillman! (second from left)



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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 $\text{fpt}(\hat{\mathbf{y}})_q, \text{fnt}(\hat{\mathbf{y}})_q$ 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, $-\infty = \tau(\hat{\mathbf{y}})_0 < \dots < \tau(\hat{\mathbf{y}})_Q = \infty$.
- 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 **Sum of Min(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 $(v_b, \Delta FP_b, \Delta FN_b, \mathcal{I}_b)$, where the $\mathcal{I}_b \in \{1, \dots, n\}$ is an example index, and there are changes $\Delta FP_b, \Delta FN_b$ 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 $\Delta FP = 0, \Delta FN = -1$, and for negative labels $y_b = -1$ we have $\Delta FP = 1, \Delta FN = 0$.
- ▶ 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

- 1: **Input:** Predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$, breakpoints in error functions $v_b, \Delta FP_b, \Delta FN_b, \mathcal{I}_b$ for all $b \in \{1, \dots, B\}$.
 - 2: Zero the $AUM \in \mathbb{R}$ and directional derivatives $\mathbf{D} \in \mathbb{R}^{n \times 2}$.
 - 3: $t_b \leftarrow v_b - \hat{y}_{\mathcal{I}_b}$ for all b .
 - 4: $s_1, \dots, s_B \leftarrow \text{SORTEDINDICES}(t_1, \dots, t_B)$.
 - 5: Compute $\underline{FP}_b, \overline{FP}_b, \underline{FN}_b, \overline{FN}_b$ for all b using s_1, \dots, s_B .
 - 6: **for** $b \in \{2, \dots, B\}$ **do**
 - 7: $AUM += (t_{s_b} - t_{s_{b-1}}) \min\{\underline{FP}_b, \overline{FN}_b\}$.
 - 8: **for** $b \in \{1, \dots, B\}$ **do**
 - 9: $\mathbf{D}_{\mathcal{I}_b, 1} += \min\{\overline{FP}_b, \overline{FN}_b\} - \min\{\overline{FP}_b - \Delta FP_b, \overline{FN}_b - \Delta FN_b\}$
 - 10: $\mathbf{D}_{\mathcal{I}_b, 2} += \min\{\underline{FP}_b + \Delta FP_b, \underline{FN}_b + \Delta FN_b\} - \min\{\underline{FP}_b, \underline{FN}_b\}$
 - 11: **Output:** AUM and matrix \mathbf{D} of directional derivatives.
- Overall $O(B \log B)$ time due to sort.