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

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Problem Setting: Maximizing Area Under ROC Curves (AUC)

My previous research on evaluating weakly supervised changepoint algorithms using AUC

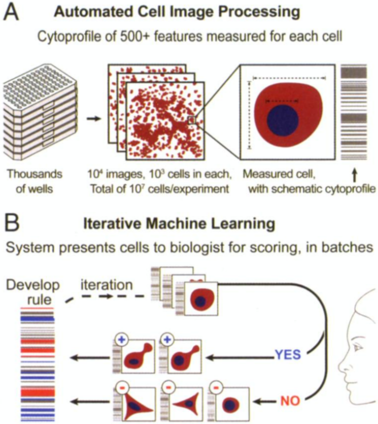
Proposed surrogate loss for ROC curve optimization

Empirical results

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 $f(\mathbf{x}) = y$?
- Example: email, $\mathbf{x}$ =bag of words, y =spam or not.
- Example: images. Jones *et al.* PNAS 2009.



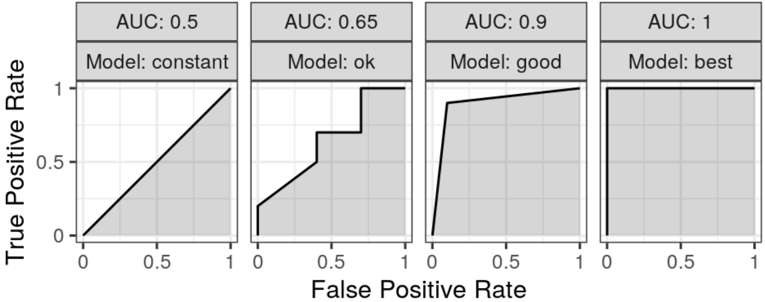
Like supervised changepoint detection, we want to minimize error rate = sum of:

False positives: $f(\mathbf{x}) = 1$ 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

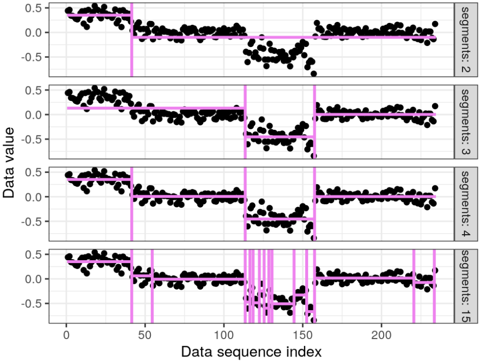
- Classic evaluation method from the signal processing literature (Egan and Egan, 1975).
- For a given set of predicted scores, plot True Positive Rate vs False Positive Rate, each point on the ROC curve is a different threshold of the predicted scores.
- Best classifier is in upper left (TPR=1, FPR=0), with large Area Under the Curve (AUC).
- Proposed idea: a new surrogate for AUC that is differentiable, so can be used for gradient descent learning.



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)

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

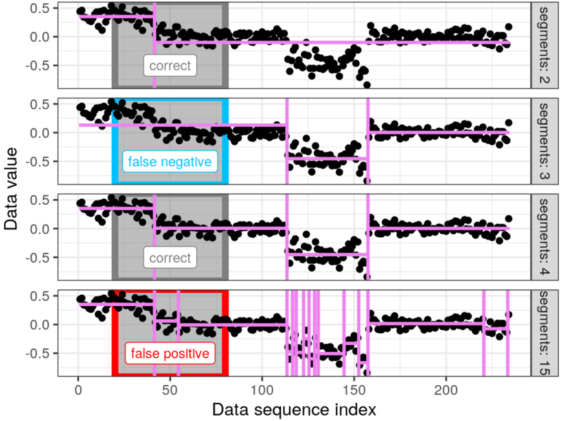


Larger penalty λ results in fewer changes/segments.

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 (sum of false positives and false negatives), or maximizes AUC.



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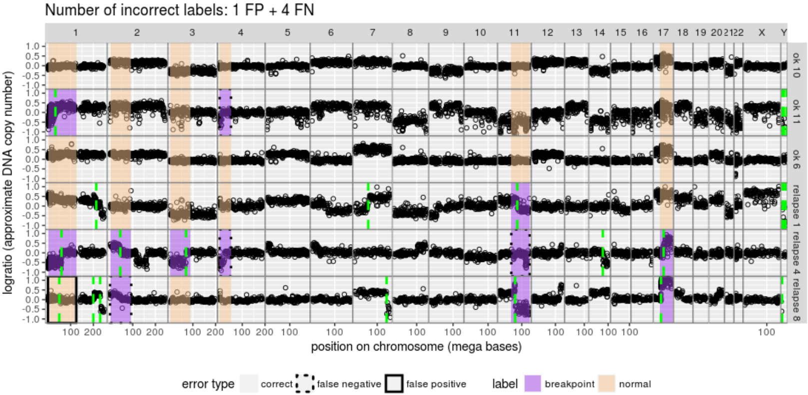
Weakly supervised changepoint detection problem setting

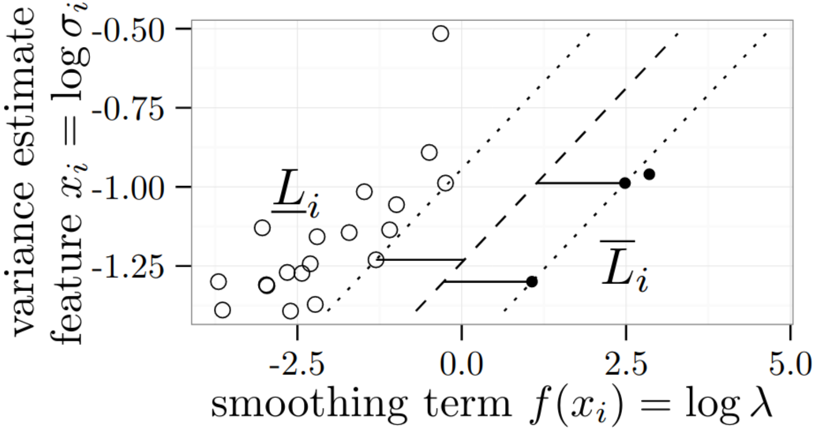
Hocking TD, Rigaill G, Bach F, Vert J-P. Learning Sparse Penalties for Change-point Detection using Max Margin Interval Regression. ICML'13.



- Black dots are data sequences in which we want to find changepoints (each panel is a separate sequence).
- Colored rectangles are weak/partial labels from an expert.
- Want accurate predictions on new/unlabeled regions.

New max-margin loss function for penalty learning

Hocking TD, Rigaill G, Bach F, Vert J-P. Learning Sparse Penalties for Change-point Detection using Max Margin Interval Regression. ICML'13.



Main new idea: learning a penalty/smoothing by minimizing a margin-based differentiable loss function (surrogate for label error), similar to Support Vector Machine and censored regression.

Empirical error rates in 10-fold cross-validation

Hocking TD, Rigaill G, Bach F, Vert J-P. Learning Sparse Penalties for Change-point Detection using Max Margin Interval Regression. ICML'13.

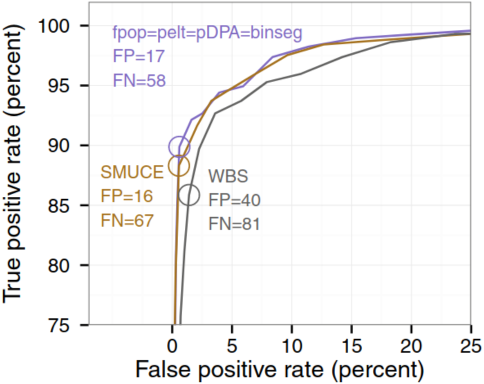
model	features m	original	high.density	low.density	simulation
BIC	0	7.99 ± 0.00	19.52 ± 0.00	13.64 ± 0.00	11.97 ± 0.00
mBIC	0	40.99 ± 0.00	70.00 ± 0.00	36.88 ± 0.00	2.25 ± 0.00
cghseg.k	0	2.19 ± 0.82	6.64 ± 3.99	6.49 ± 1.16	11.85 ± 3.52
log.d	1	2.40 ± 1.00	7.59 ± 6.43	6.21 ± 1.01	13.13 ± 4.14
log.s.log.d	2	1.90 ± 0.77	8.12 ± 5.62	4.72 ± 0.54	1.50 ± 1.63
L1-reg	117	1.81 ± 0.58	7.66 ± 5.72	4.70 ± 0.88	1.28 ± 1.47

Proposed penalty learning methods ($m \geq 1$ features with linear weights to learn) have much smaller error rates than previous unsupervised models (BIC, mBIC) and constant method (cghseg.k).

Empirical evaluation using AUC

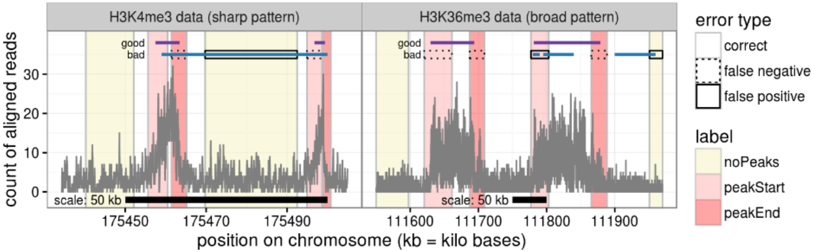
Maidstone R, Hocking TD, Rigaill G, Fearnhead P. On optimal multiple changepoint algorithms for large data. Statistics and Computing (2016).

- Proposed fpop, a fast new algorithm for computing optimal solution to penalized changepoint problem.
- Prediction accuracy analysis using AUC in labeled neuroblastoma data set.



Weakly supervised peak detection in genomic data

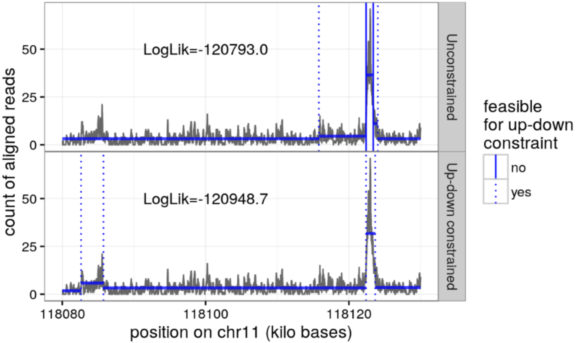
Hocking TD, Rigaill G, Fearnhead P, Bourque G. Constrained Dynamic Programming and Supervised Penalty Learning Algorithms for Peak Detection in Genomic Data. Journal of Machine Learning Research 21(87):1-40, 2020.



Problem setting: weakly supervised peak detection in genomic data (want to learn peak pattern from partial labels, and predict consistently/accurately in unlabeled regions).

New up-down constraints on adjacent segment means

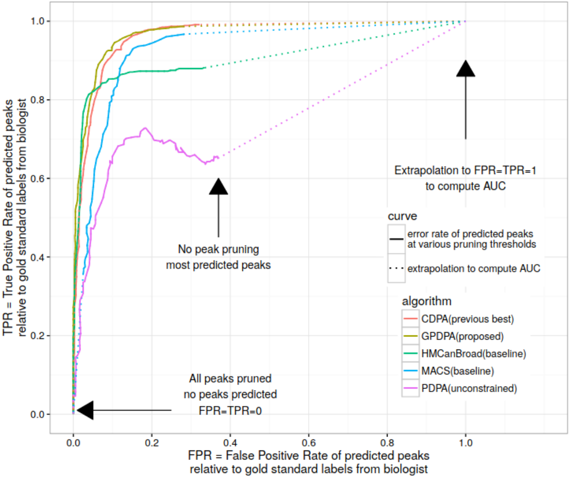
Hocking TD, Rigaill G, Fearnhead P, Bourque G. Constrained Dynamic Programming and Supervised Penalty Learning Algorithms for Peak Detection in Genomic Data. Journal of Machine Learning Research 21(87):1-40, 2020.



Proposed fast dynamic programming algorithm for computing optimal changepoints subject to up-down constraints on adjacent segment means.

Evaluating peak detection algorithms using AUC

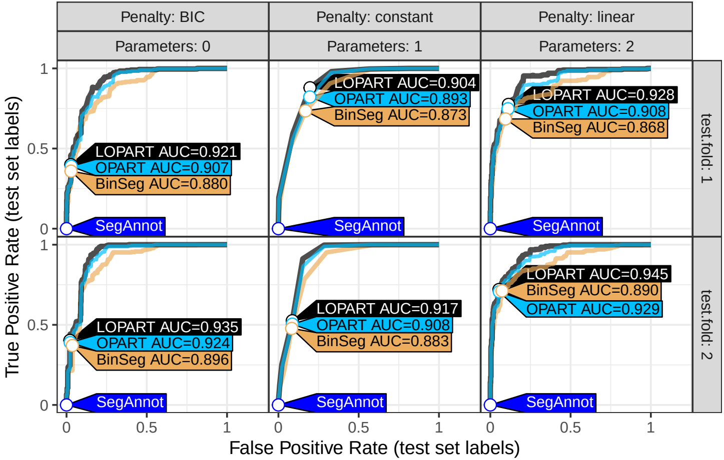
Hocking TD, Rigaill G, Fearnhead P, Bourque G. Constrained Dynamic Programming and Supervised Penalty Learning Algorithms for Peak Detection in Genomic Data. Journal of Machine Learning Research 21(87):1-40, 2020.



Proposed GPDPA has larger AUC than previous algorithms.

Evaluating a new algorithm with label constraints

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



Proposed LOPART algorithm has consistently larger test AUC than previous algorithms.

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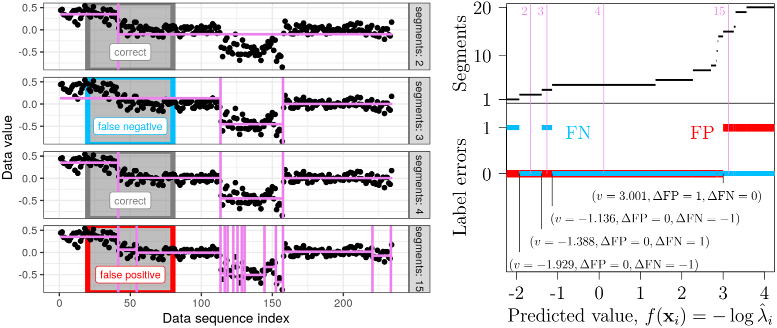
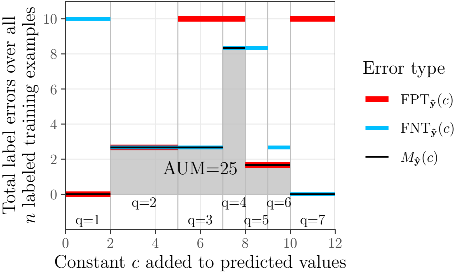
Changepoint FP/FN functions may be non-monotonic

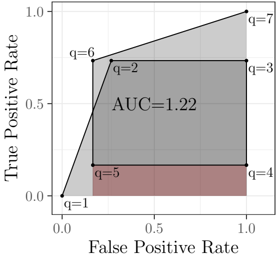


- Optimal changepoint model may have non-monotonic error (for example FN), because changepoints at model size s may not be present in model $s+1$.
- Penalty values where the FP/FN changes can be efficiently computed. Hocking TD, Vargovich J. Linear Time Dynamic Programming for Computing Breakpoints in the Regularization Path of Models Selected From a Finite Set. Journal of Computational and Graphical Statistics (2021).

Looping ROC curve, simple synthetic example

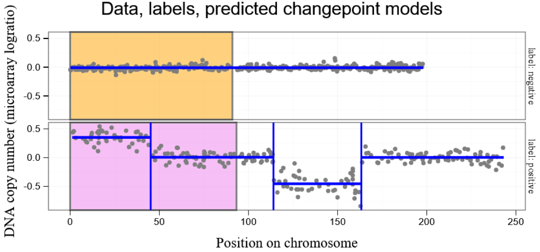
- Non-monotonic FP/FN can result in looping ROC curve.
- AUC can be greater than one (dark grey area double counted, red area negative counted).
- Loops have very sub-optimal points (large min error, for example q=4), so do we want to maximize AUC?
- Minimize Area Under Min (AUM) instead, which encourages monotonic ROC curve with points in upper left (small min error, for example q=1,6,7).





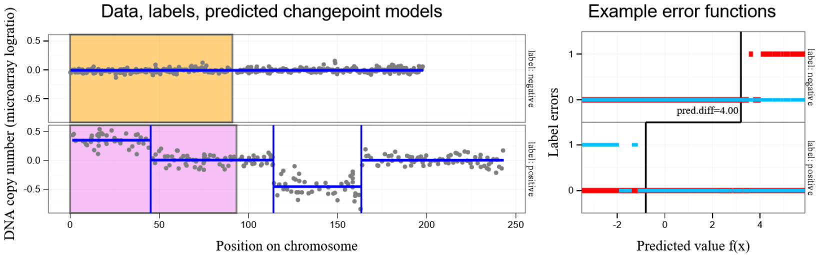
Two real data sets

https://bl.ocks.org/tdhock/raw/545d76ea8c0678785896e7dbe5ff5510/



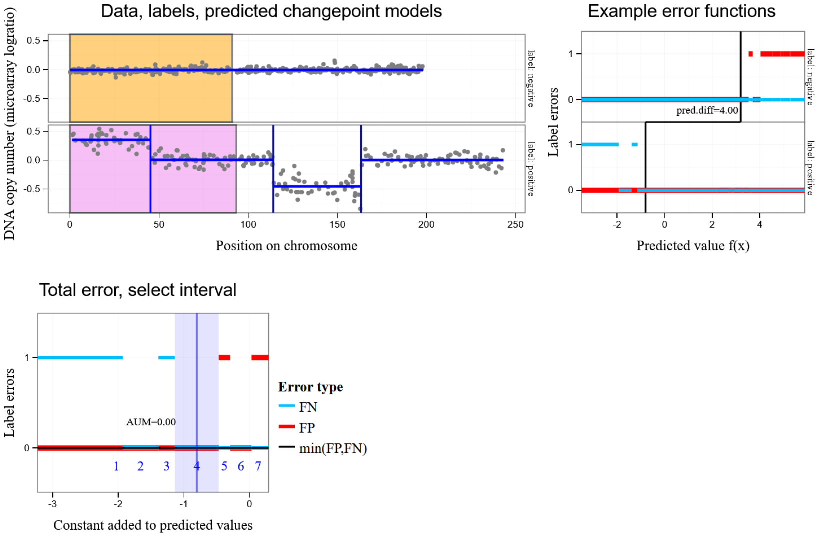
Two real error functions

https://bl.ocks.org/tdhock/raw/545d76ea8c0678785896e7dbe5ff5510/



Total error as a function of constant added to predictions

https://bl.ocks.org/tdhock/raw/545d76ea8c0678785896e7dbe5ff5510/



Corresponding ROC curves

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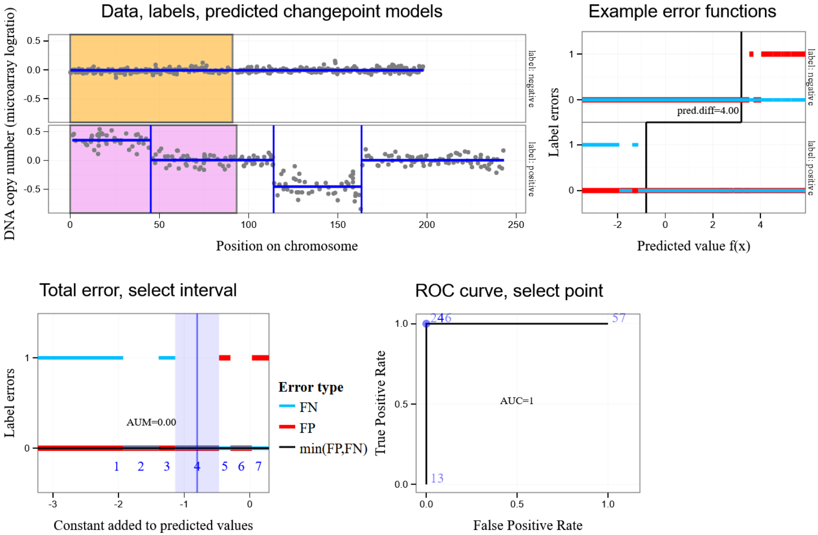
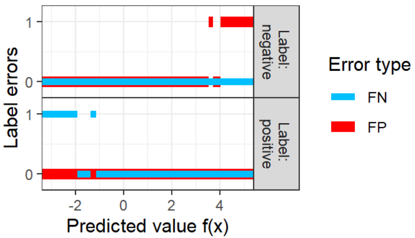
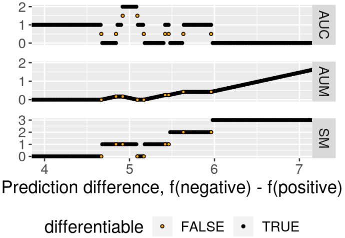


Real data example with AUC greater than one

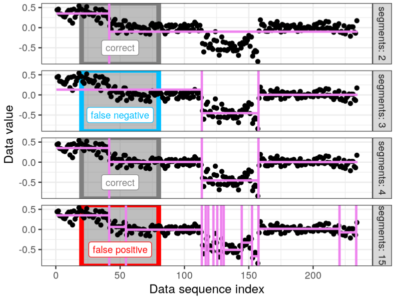


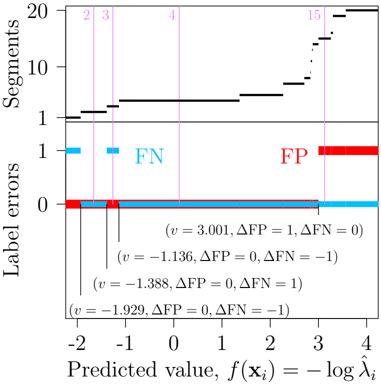


- $n = 2$ labeled changepoint problems.
- AUC=2 when prediction difference=5.
- AUM=0 implies AUC=1.
- AUM is continuous L1 relaxation of non-convex Sum of Min (SM).
- AUM is differentiable almost everywhere.
- Main new idea: compute the gradient of this function and use it for learning.

Algorithm inputs: predictions and label error functions

- Each observation $i \in \{1, \dots, n\}$ 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 $\mathcal{I}_b \in \{1, \dots, n\}$.



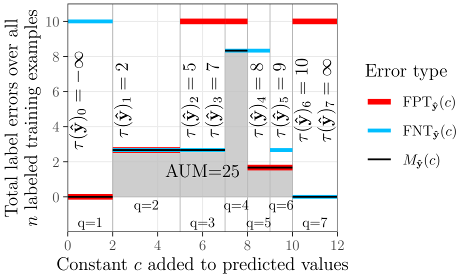


Algorithm computes total FP and FN for each threshold/constant added to predicted values

- 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:

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

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



Algorithm computes two directional derivatives

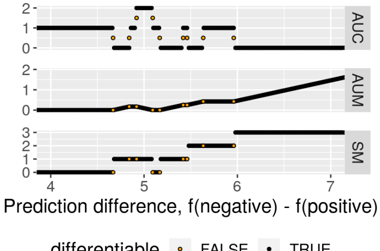
- Gradient only defined when function is differentiable, but AUM is not differentiable everywhere (see below).
- Directional derivatives defined everywhere.

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

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

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

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



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

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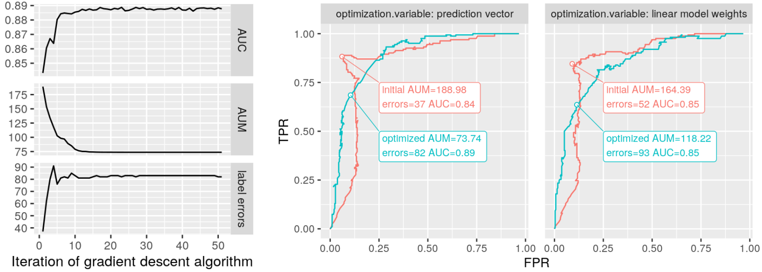
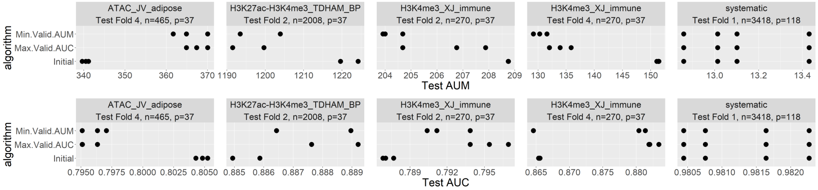
AUM gradient descent results in increased train AUC for a real changepoint problem



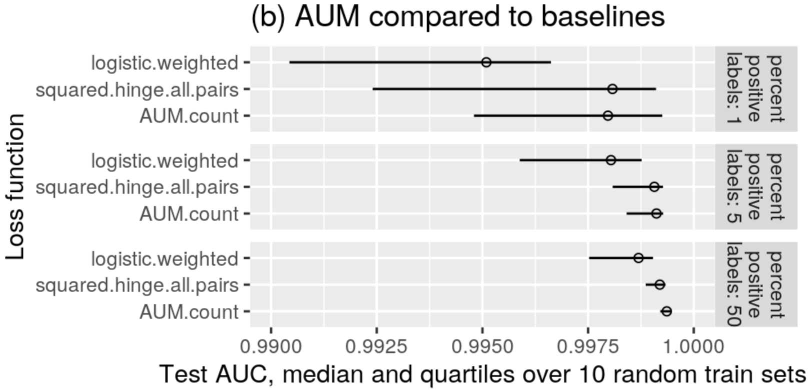
- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), gradient descent on weight vector.

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



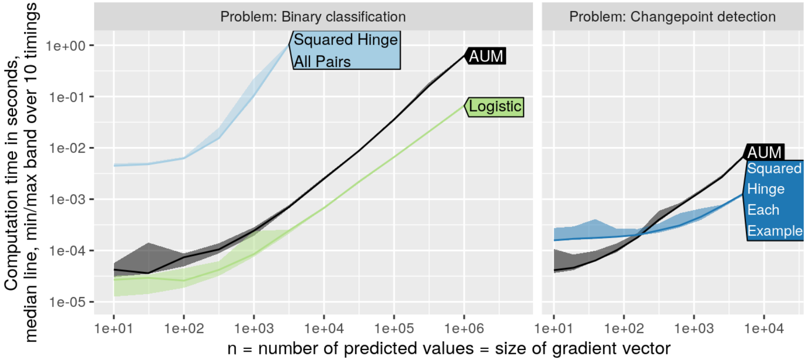
- Five changepoint problems (panels from left to right).
- Two evaluation metrics (AUM=top, AUC=bottom).
- Three algorithms (Y axis), Initial=Min regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), Min.Valid.AUM/Max.Valid.AUC=AUM gradient descent with early stopping regularization.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

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

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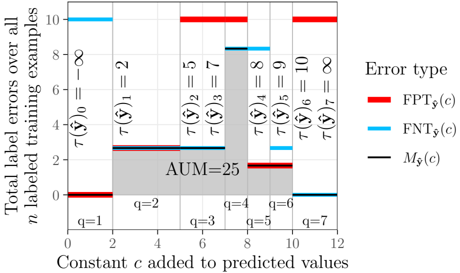
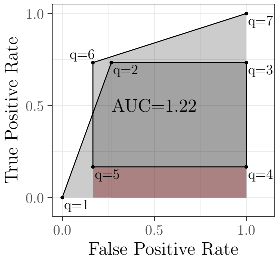
More notation

- 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 $\text{fpt}(\hat{\mathbf{y}})_q, \text{fpt}(\hat{\mathbf{y}})_q$ 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 a continuous 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

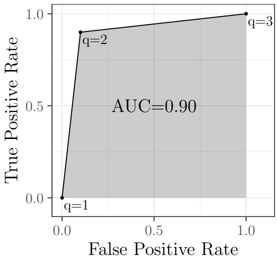
Input: Predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$, breakpoints in error functions $v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b$ for all $b \in \{1, \dots, B\}$.
Zero the AUM $\in \mathbb{R}$ and directional derivatives $\mathbf{D} \in \mathbb{R}^{n \times 2}$.
$t_b \leftarrow v_b - \hat{y}_{\mathcal{I}_b}$ 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**
    $\mathbf{D}_{\mathcal{I}_b,1} += \min\{\overline{\text{FP}}_b, \overline{\text{FN}}_b\} - \min\{\overline{\text{FP}}_b - \Delta\text{FP}_b, \overline{\text{FN}}_b - \Delta\text{FN}_b\}$
    $\mathbf{D}_{\mathcal{I}_b,2} += \min\{\underline{\text{FP}}_b + \Delta\text{FP}_b, \underline{\text{FN}}_b + \Delta\text{FN}_b\} - \min\{\underline{\text{FP}}_b, \underline{\text{FN}}_b\}$
Output: AUM and matrix $\mathbf{D}$ of directional derivatives.

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

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).

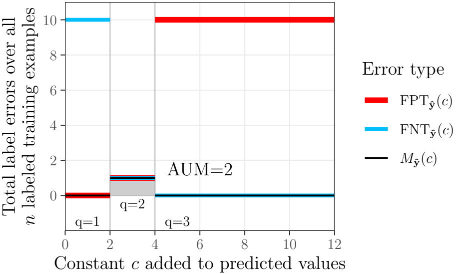


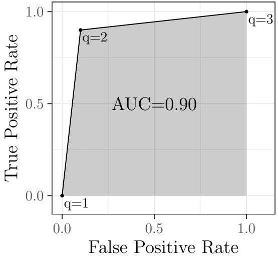
In binary classification, ROC curve is monotonic increasing.

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

Area Under ROC curve, synthetic example

- Labels = [1,0,0,...,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, $q = 3$.

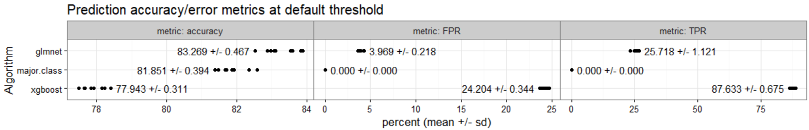




Real data example when ROC curves are useful

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?



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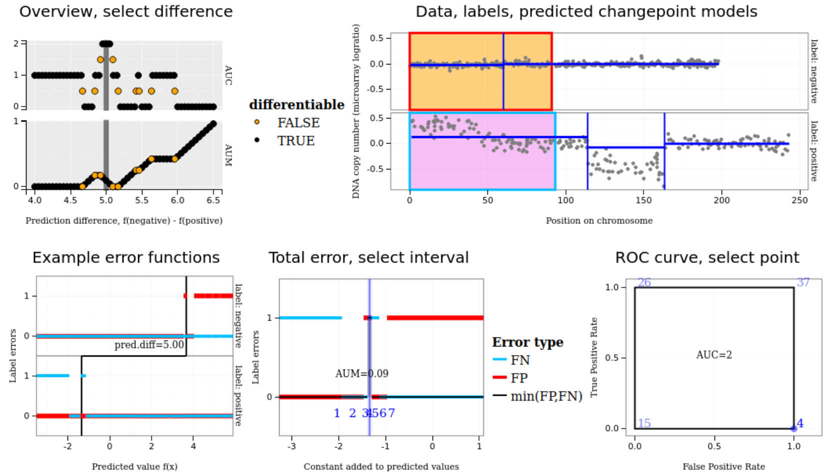
Real data example, interactive AUC/AUM demo



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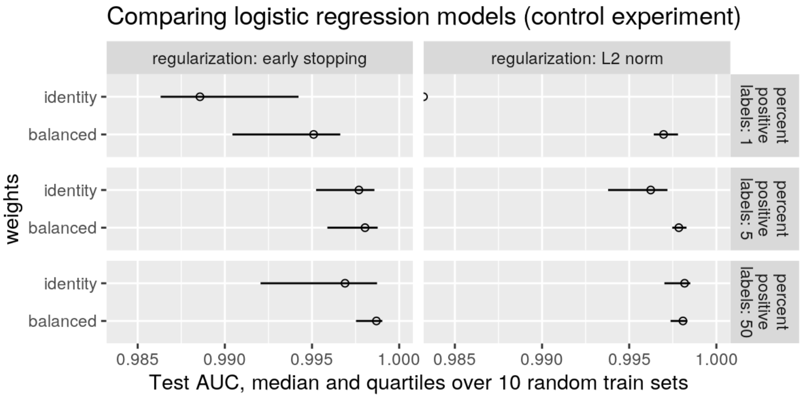
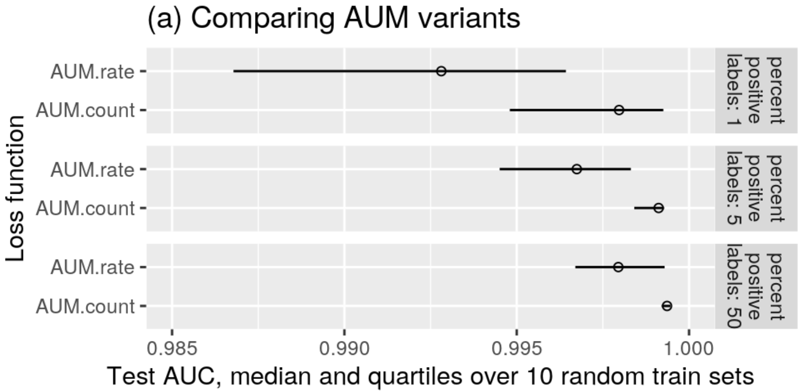
Standard logistic loss fails for highly imbalanced labels



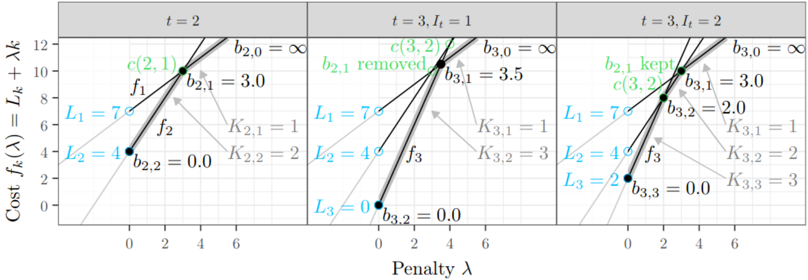
- Subset of zip.train/zip.test data (only 0/1 labels).
- Test set size 528 with balanced labels (50%/50%).
- Train set size 1000 with variable class imbalance.
- Loss is $\ell[f(x_i), y_i]w_i$ with $w_i = 1$ for identity weights, $w_i = 1/N_{y_i}$ for balanced, ex: 1% positive means $w_i \in \{1/10, 1/990\}$.

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.

DP model selection TODO



DP model selection TODO