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

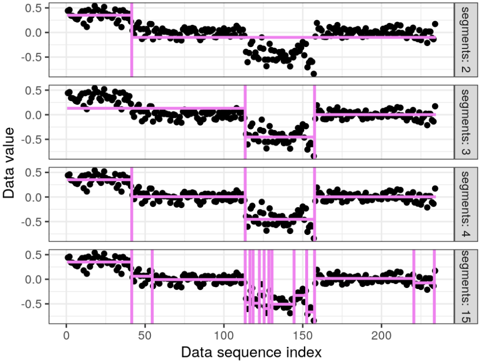
Empirical results

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)

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

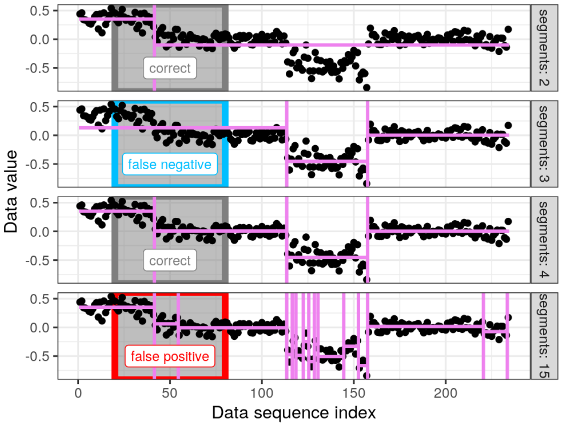


Larger penalty λ results in fewer changes/segments.

Smaller penalty λ results in more changes/segments.

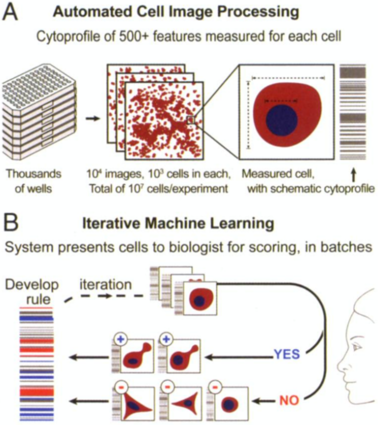
Problem: weakly supervised changepoint detection

- 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.

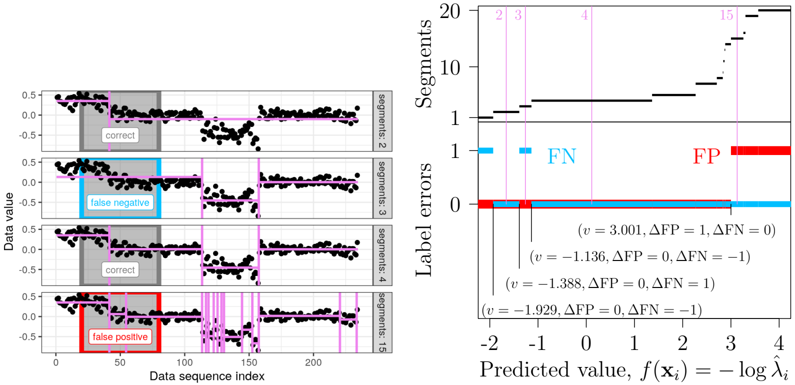


Like supervised changepoint detection, we want to minimize error rate = sum of:

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).

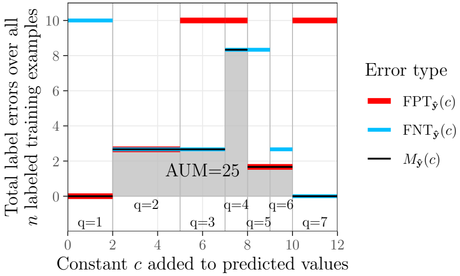
Real changepoint problem with non-monotonic label error

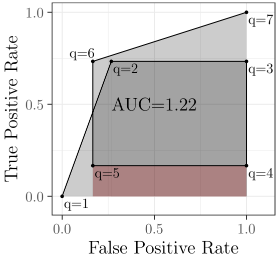


Optimal changepoint model may have non-monotonic error (for example FN), because changepoints at model size s may not be present in model $s + 1$.

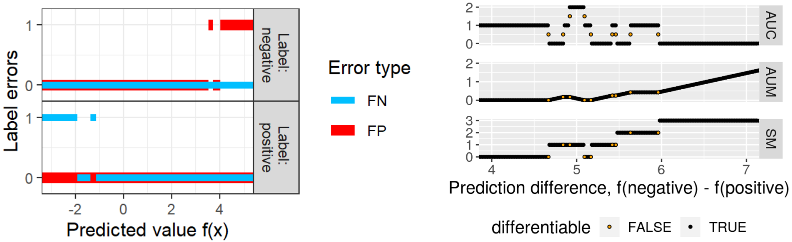
Looping ROC curve, simple synthetic example

- 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).





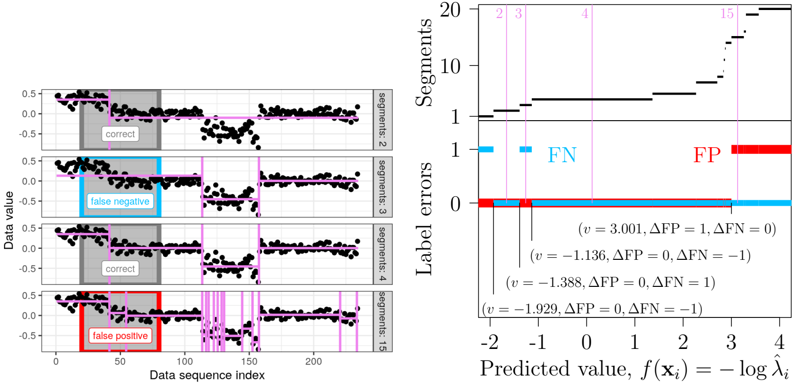
Real data example with AUC greater than one



- $n = 2$ 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 $i \in \{1, \ldots, n\}$ has a predicted value $\hat{y}_i \in \mathbb{R}$.
- Breakpoints $b \in \{1, \ldots, B\}$ used to represent label error via tuple $(v_b, \Delta FP_b, \Delta FN_b, \mathcal{I}_b)$.
- There are changes $\Delta FP_b, \Delta FN_b$ at predicted value $v_b \in \mathbb{R}$ in error function $\mathcal{I}_b \in \{1, \ldots, n\}$.

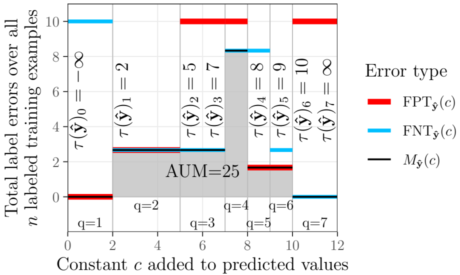


Algorithm computes total FP and FN for each threshold/constant added to predicted values

- 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:

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

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



Algorithm computes two directional derivatives

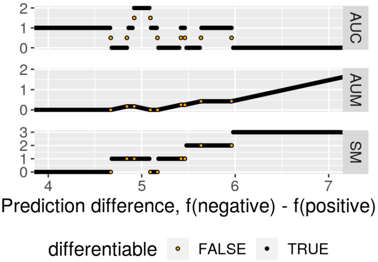
- Gradient only defined when function is differentiable, but AUM is not differentiable everywhere (see below).
- Directional derivatives defined everywhere.

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

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

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

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



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

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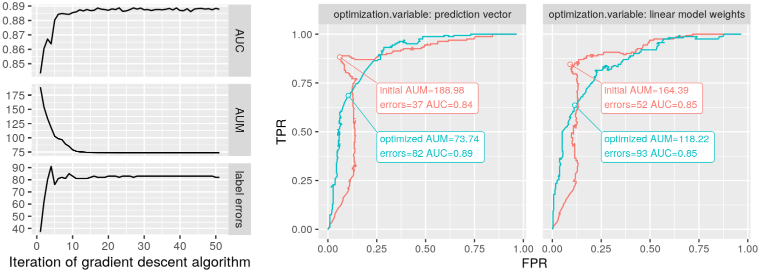
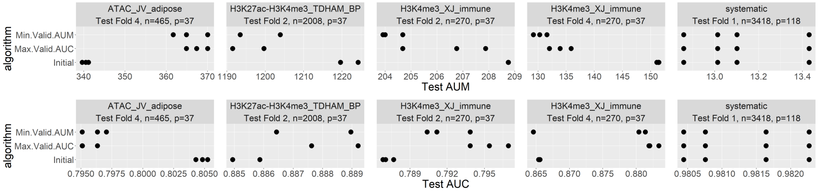
AUM gradient descent results in increased train AUC for a real changepoint problem



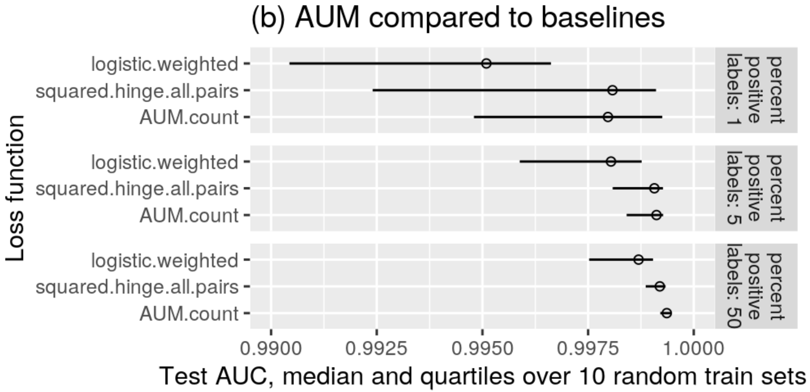
- Left/middle: changepoint problem initialized to prediction vector with min label errors, gradient descent on prediction vector.
- Right: linear model initialized by minimizing regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), gradient descent on weight vector.

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



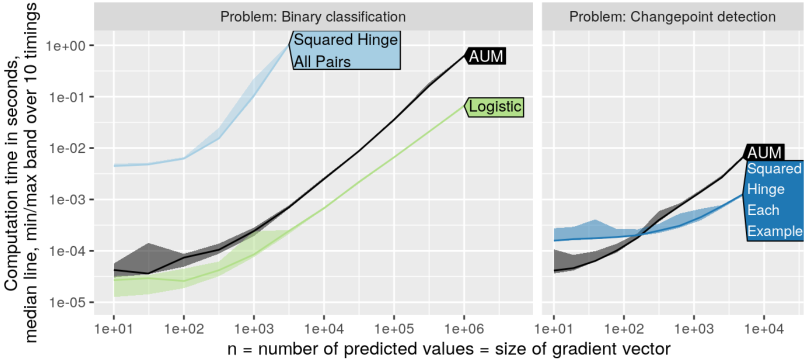
- Five changepoint problems (panels from left to right).
- Two evaluation metrics (AUM=top, AUC=bottom).
- Three algorithms (Y axis), Initial=Min regularized convex loss (surrogate for label error, Hocking *et al.* ICML 2013), Min.Valid.AUM/Max.Valid.AUC=AUM gradient descent with early stopping regularization.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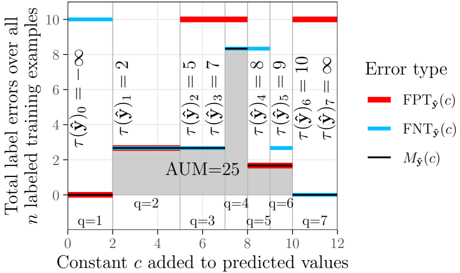
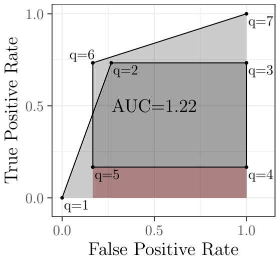
More notation

- 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

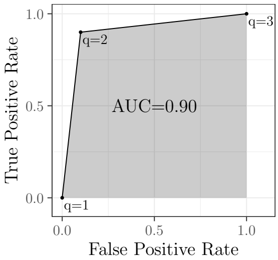
Input: Predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$, breakpoints in error functions $v_b, \Delta\text{FP}_b, \Delta\text{FN}_b, \mathcal{I}_b$ for all $b \in \{1, \dots, B\}$.
Zero the AUM $\in \mathbb{R}$ and directional derivatives $\mathbf{D} \in \mathbb{R}^{n\times 2}$.
$t_b \leftarrow v_b - \hat{y}_{\mathcal{I}_b}$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

- 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).

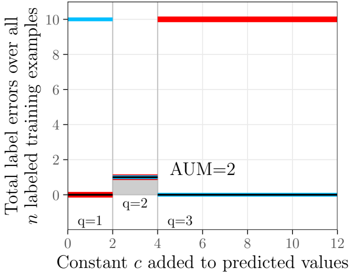


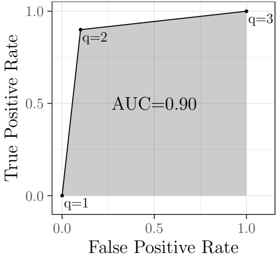
In binary classification, ROC curve is monotonic increasing.

- 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, $q = 3$.

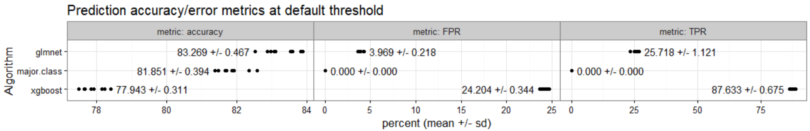




Real data example when ROC curves are useful

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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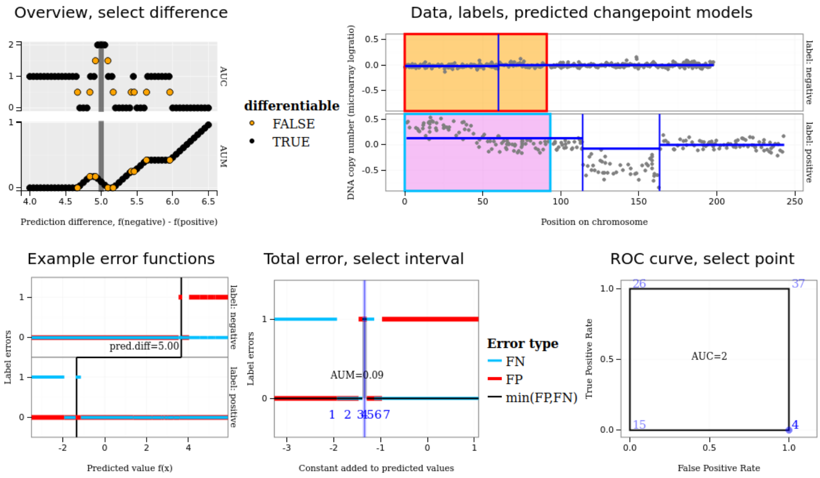
Real data example, interactive AUC/AUM demo



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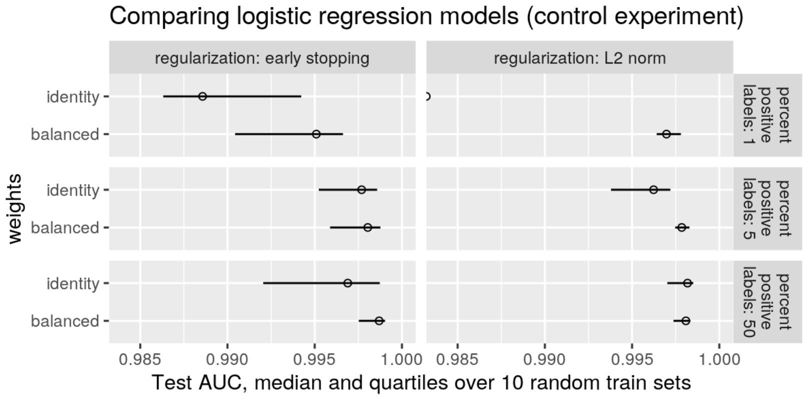
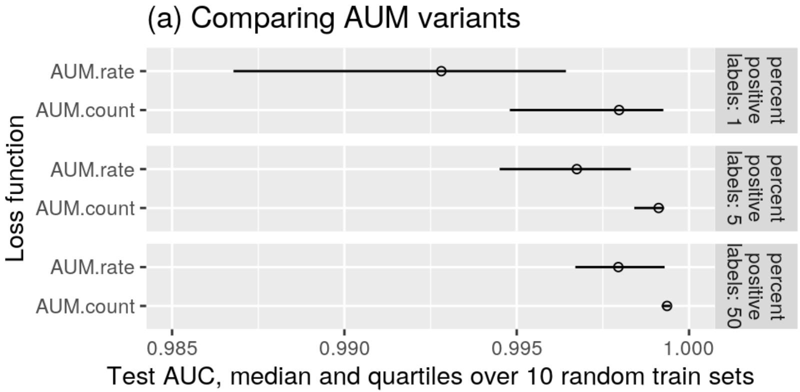
Standard logistic loss fails for highly imbalanced labels



- 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.