

Algorithmes efficaces pour la détection de ruptures

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Brief history of optimal change-point algorithms

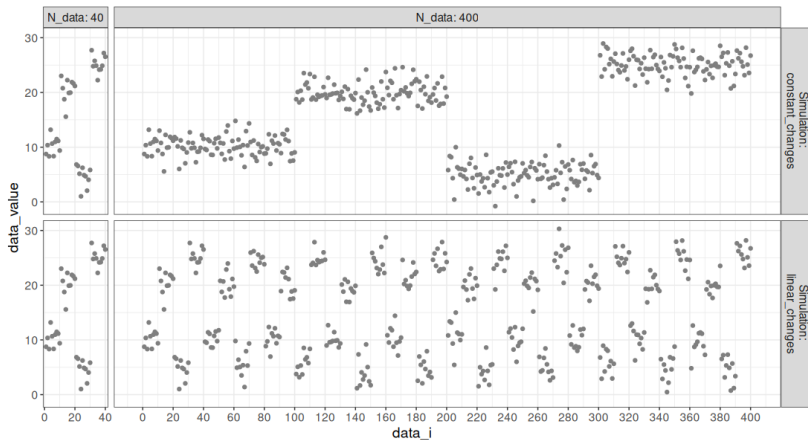
New algorithms with constraints between adjacent segments

Computing optimal changepoints subject to label constraints

Learning to predict the number of changepoints

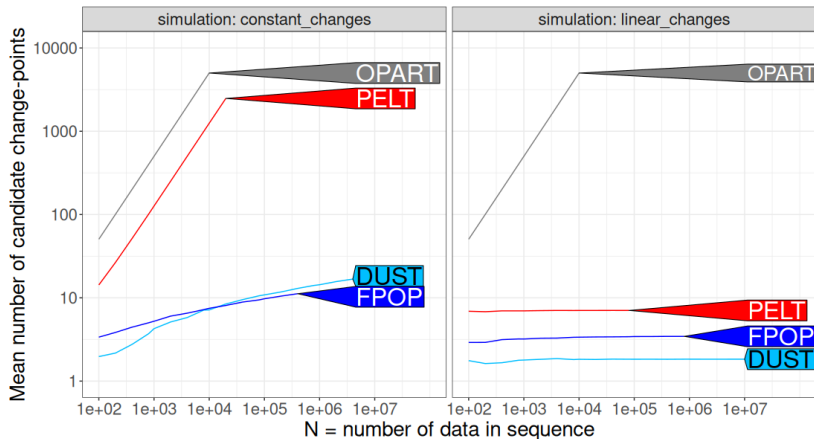
Summary and Discussion

Simulated data with constant and linear changes



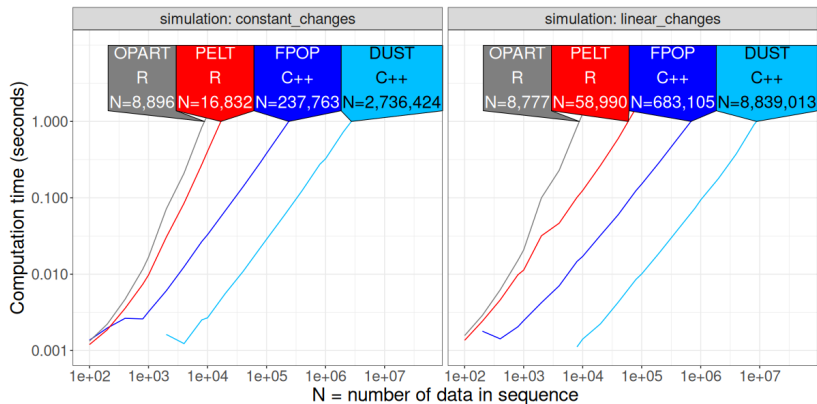
<https://tdhock.github.io/blog/2025/PELT-vs-fpopw/>

Number of candidates considered



<https://tdhock.github.io/blog/2025/PELT-vs-fpopw/>

Overall computation time



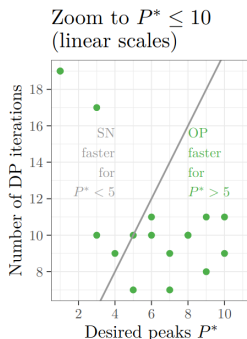
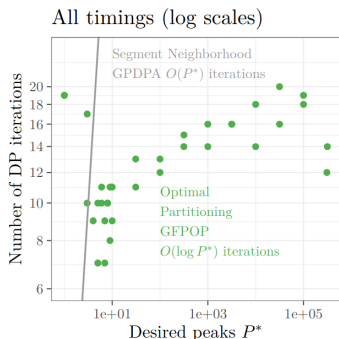
<https://tdhock.github.io/blog/2025/PELT-vs-fpopw/>

Computing various solutions using penalized solver

How to compute the best model with a given number P^* of change-points?

- ▶ Example: $P^* = 100$ change-points?
- ▶ Could run constrained solver to get all models from 0 to P^* change-points.
- ▶ Required number of DP iterations is linear in number of change-points, $O(P^*)$ —slow if P^* large.
- ▶ Penalized solver returns best change-points for a given penalty $\lambda \geq 0$ (but λ that yields P^* is unknown).
- ▶ Sequential search: Hocking *et al.*, Journal of Statistical Software 101(10) (2022).
- ▶ DP iterations logarithmic in number of change-points, $O(\log P^*)$ —fast for large P^* !

Penalized (OP) is faster than constrained (SN)



- ▶ Figure: genomic data, $N \approx 10^6$,
- ▶ Sequential search repeated runs penalized (OP) solver.
- ▶ Example: for $N = 10^7$, desired change-points $P^* = 3000$.
- ▶ Constrained (SN) solver: 100TB storage, 10 weeks.
- ▶ Penalized (OP) solver: 100GB storage, 10 hours.

Hocking *et al.*, Journal of Statistical Software 101(10) (2022).

Computing ranges of solutions using penalized solver

How to compute all models with penalties $\lambda \in [\underline{\lambda}, \overline{\lambda}]$?

- ▶ Example: $\lambda \in [0.1, \overline{10.5}]$?
- ▶ CROPS: Change-points for a Range Of Penalties.
- ▶ Haynes, *et al.* Journal of Computational and Graphical Statistics, 26(1), 134-143 (2017).

How to compute all models with number of change-points $P \in [\underline{P}, \overline{P}]$?

- ▶ Example: all models from 50 to 60 change-points?
- ▶ CROCS: Change-points for a Range Of Complexities.
- ▶ Liehrmann *et al.*, BMC Bioinformatics 22(323) (2021).

If M is the number of models to compute (ex: 11 models from 50 to 60 change-points), then $O(M + \log \overline{P})$ DP iterations—fast for large model sizes \overline{P} .

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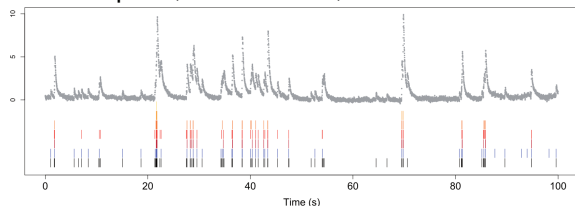
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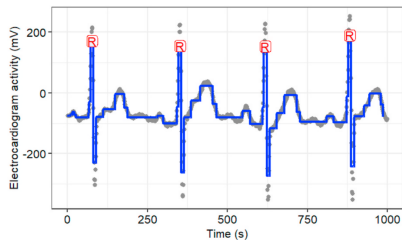
Summary and Discussion

Changepoint detection algorithms for data over time

Neuron spikes, Jewell *et al.*, Biostatistics 2019.

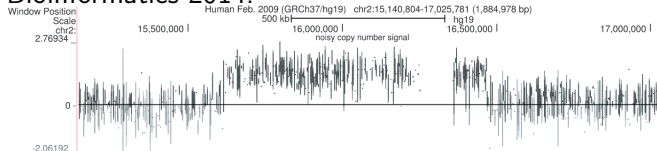


Electrocardiograms (heart monitoring), Fotoohinasab *et al.*, Asilomar conference 2020.

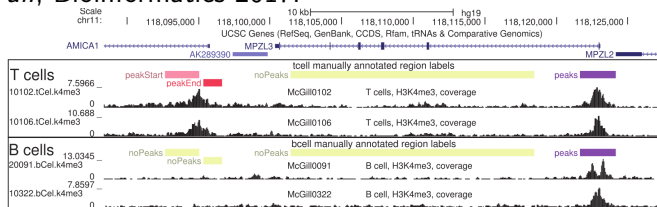


Changepoint detection algorithms for data over space

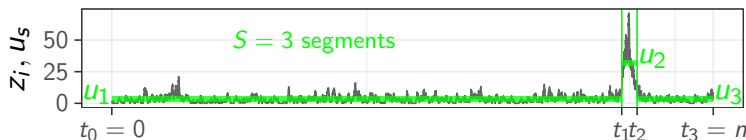
DNA copy number data for cancer diagnosis, Hocking *et al.*, Bioinformatics 2014.



ChIP-seq data for understanding the human genome, Hocking *et al.*, Bioinformatics 2017.



Optimal changepoint detection problem and algorithms



$$\min_{\substack{\mathbf{u} \in \mathbb{R}^S \\ 0=t_0 < t_1 < \dots < t_{S-1} < t_S=n}} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i)$$

- ▶ Algorithm inputs n data z_1, \dots, z_n and $\#$ of segments S .
- ▶ Goal is to compute best $S - 1$ changepoints $t_1 < \dots < t_{S-1}$ and S segment parameters u_1, \dots, u_S .
- ▶ Hard non-convex optimization problem, naïvely $O(n^S)$ time.
- ▶ Auger and Lawrence 1989: $O(Sn^2)$ time algorithm.
- ▶ Rigaiil 2015: $O(n \log n)$ time, change in any direction.
- ▶ Hocking *et al.*, 2020: $O(n \log n)$, directional constraints.

Constrained optimization algorithm speed

Hocking *et al.*, Journal of Machine Learning Research 2020.

$$\begin{aligned} & \min_{\substack{\mathbf{u} \in \mathbb{R}^S \\ 0=t_0 < t_1 < \dots < t_{S-1} < t_S=n}} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i) \\ & \text{subject to} \quad u_{s-1} \leq u_s \quad \forall s \in \{2, 4, \dots\}, \\ & \quad \quad \quad u_{s-1} \geq u_s \quad \forall s \in \{3, 5, \dots\}. \end{aligned}$$

Constraints used to force change up to peak state, then change down to background noise state.

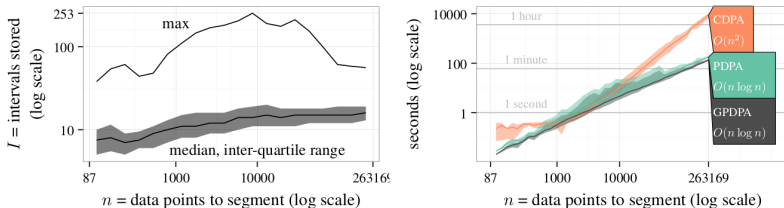
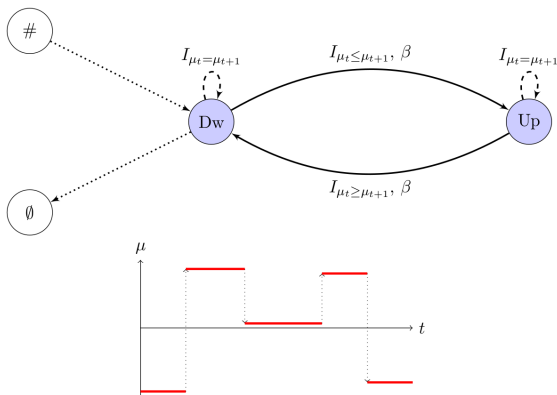


Figure 3: Empirical speed analysis on 2752 count data vectors from the histone mark ChIP-seq benchmark. For each vector we ran the GPDPA with the up-down constraint and a max of $K = 19$ segments. The expected time complexity is $O(KnI)$ where I is the average number of intervals (function pieces; candidate changepoints) stored in the $C_{k,t}$ cost functions. **Left:** number of intervals stored is $I = O(\log n)$ (median, inter-quartile range, and maximum over all data points t and segments k). **Right:** time complexity of the GPDPA is $O(n \log n)$ (median line and min/max band).

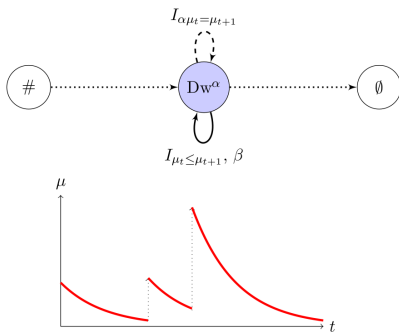
Optimization constraints defined using a graph

Runge *et al.*, Journal of Statistical Software 2023 (graph figures).

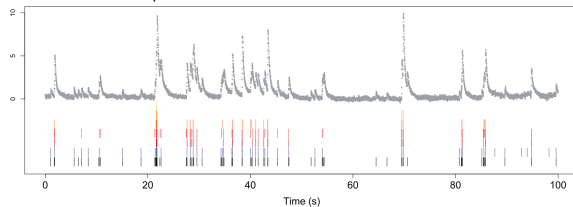


- ▶ Purple Dw/Up nodes represent hidden states.
- ▶ #/∅ nodes constrain start/end state.
- ▶ Edges represent possible state transitions.
- ▶ gfpop R package with C++ code computes optimal changepoints for user-defined constraint graphs.

All up changes, exponentially decaying segments



Jewell *et al.*, Biostatistics 2019.



References

- ▶ Auger IE and Lawrence CE. Algorithms for the optimal identification of segment neighborhoods. *Bull Math Biol* 51:39–54 (1989).
- ▶ G Rigaiil. A pruned dynamic programming algorithm to recover the best segmentations with 1 to kmax change-points. *Journal de la Société Française de la Statistique*, 156(4), 2015.
- ▶ **Hocking TD**, Boeva V, Rigaiil G, Schleiermacher G, Janoueix-Lerosey I, Delattre O, Richer W, Bourdeaut F, Suguro M, Seto M, Bach F, Vert J-P. SegAnnDB: interactive Web-based genomic segmentation. *Bioinformatics* (2014) 30 (11): 1539-1546.
- ▶ **Hocking TD**, Goerner-Potvin P, Morin A, Shao X, Pastinen T, Bourque G. Optimizing ChIP-seq peak detectors using visual labels and supervised machine learning. *Bioinformatics* (2017) 33 (4): 491-499.
- ▶ Jewell S, **Hocking TD**, Fearnhead P, Witten D. Fast Nonconvex Deconvolution of Calcium Imaging Data. *Biostatistics* (2019).
- ▶ Fotoohinasab A, **Hocking TD**, Afghah F. A Graph-Constrained Changepoint Learning Approach for Automatic QRS-Complex Detection. *Asilomar Conference on Signals, Systems, and Computers* (2020).
- ▶ **Hocking TD**, Rigaiil 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.
- ▶ Runge V, **Hocking TD**, Romano G, Afghah F, Fearnhead P, Rigaiil G. gfpop: an R Package for Univariate Graph-Constrained Change-point Detection. *Journal of Statistical Software* 106(6) (2023).

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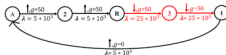
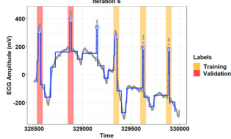
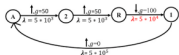
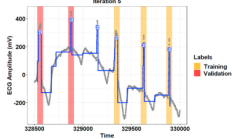
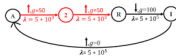
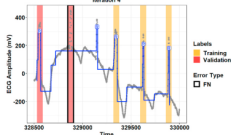
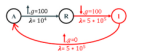
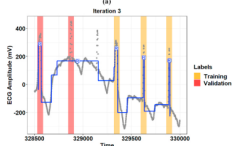
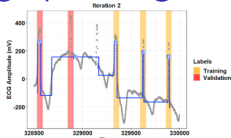
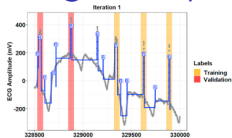
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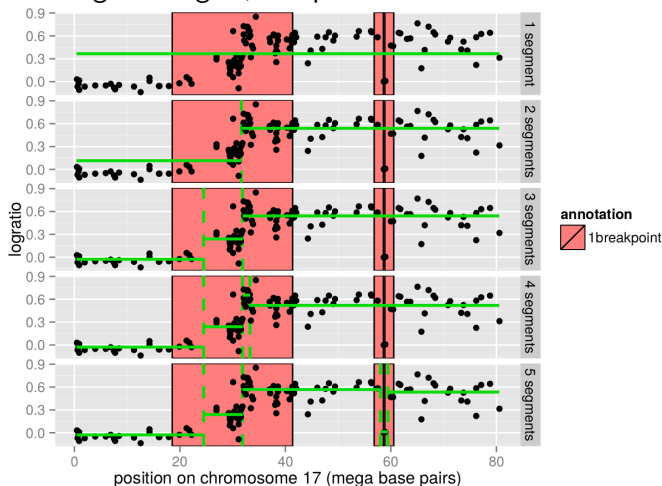
Learning a complex graph using labels



- Fotoohinasab *et al.*, 2021.
- Simple initial graph is iteratively edited (red) to agree with expert labeled regions (orange rectangles).
- Easier for expert to provide labels than graph.

What if no models agree with expert labels?

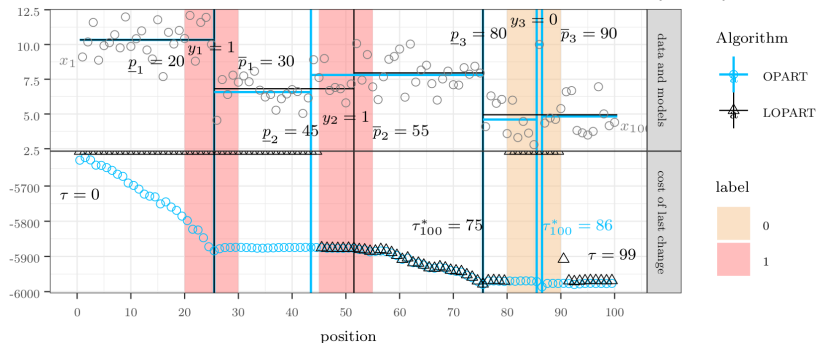
Hocking and Rigai, Pre-print hal-00759129.



- ▶ Expert wants: one changepoint in each label (red rectangle).
- ▶ No model is consistent with all three labels.

Using expert labels as optimization constraints

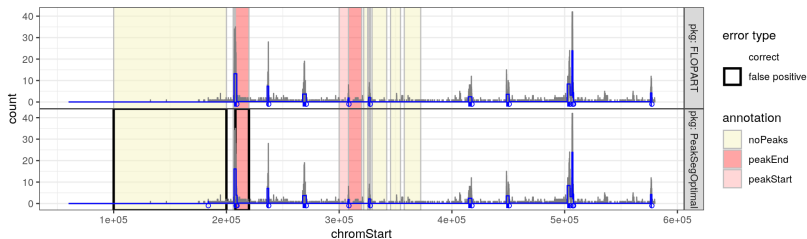
Hocking and Srivastava, Computational Statistics 38 (2023).



- ▶ Previous OPART model (blue) ignores y_3 labels (two errors).
- ▶ Main idea: add optimization constraints to ensure that there is the right number of changepoints predicted in each label.
- ▶ Proposed LOPART model (black) consistent with labels.

Label constraints and directional constraints

Stenberg and Hocking, in progress.



- ▶ Previous PeakSegOptimal algorithm (bottom) ignores labels (two errors).
- ▶ Proposed FLOPART model (top) consistent with labels, and interpretable in terms of up changes to peaks and down changes to background noise.

References

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- ▶ **Hocking TD**, Srivastava A. Labeled Optimal Partitioning. Computational Statistics 38 (2023).
- ▶ Fotoohinasab A, **Hocking TD**, Afghah F. A Greedy Graph Search Algorithm Based on Changepoint Analysis for Automatic QRS-Complex Detection. Computers in Biology and Medicine 130 (2021).

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How to predict the number of changes?

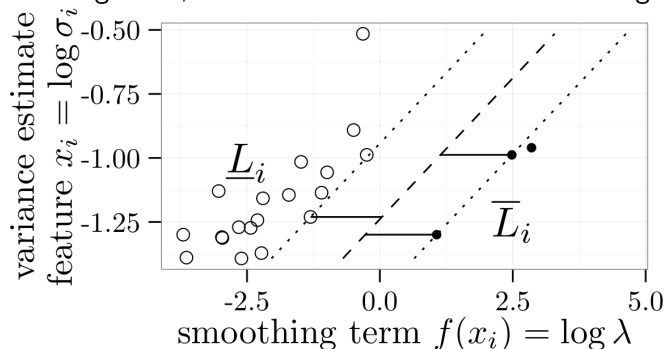
We assumed that the number of segments S is provided as an input parameter to our optimization algorithm.

$$\min_{\substack{\mathbf{u} \in \mathbb{R}^S \\ 0=t_0 < t_1 < \dots < t_{S-1} < t_S=n}} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i)$$

In practice S is often unknown — what value should we use?

Learning to predict number of changes similar to SVM

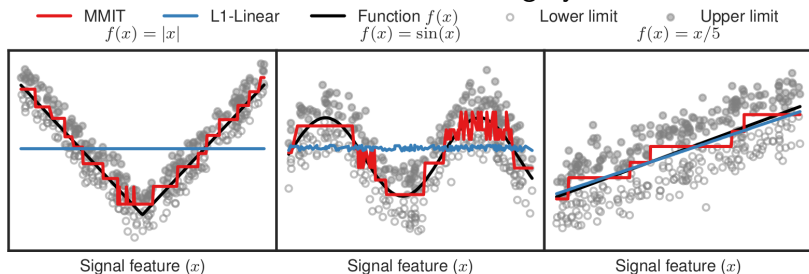
Hocking *et al.*, Int'l Conference on Machine Learning 2013.



- ▶ Train on several data sequences with labels (dots).
- ▶ Want to compute function between white and black dots.
- ▶ SVM margin is multi-dimensional (diagonal).
- ▶ Here margin to maximize is one-dimensional (horizontal).
- ▶ Learned function predicts number of changepoints/segments.

Decision tree learns non-linear function of inputs

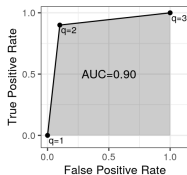
Drouin *et al.*, Neural Information Processing Systems 2017.



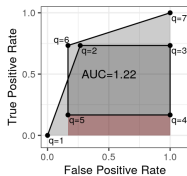
- ▶ Generalization of classical CART regression tree learning algorithm.
- ▶ Can learn non-linear functions of inputs.
- ▶ More recently we implemented a similar idea in xgboost, Barnwal *et al.*, Journal of Computational and Graphical Statistics 31(4) (2022).

Is maximizing Area Under the ROC Curve desirable?

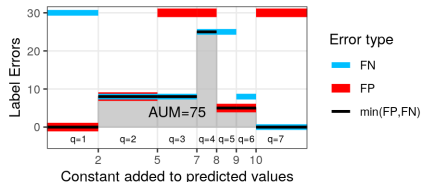
In binary classification the ROC curve is monotonic.



In changepoint detection it can have loops.

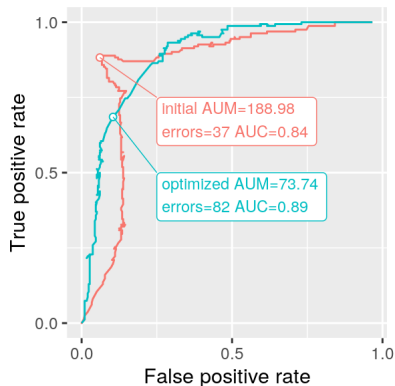
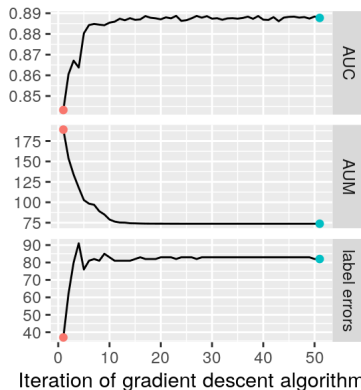


We propose instead to minimize the $AUM = \text{Area Under the Minimum of false positives and false negatives}$, as a function of prediction threshold.



AUM gradient descent algorithm optimizes AUC

Hillman and Hocking, in progress.



- ▶ Initial predictions: minimum label errors.
- ▶ ROC curves become more regular/monotonic after optimization, but label error increases.
- ▶ Trade-off between AUC and label error optimization that does not exist in binary classification.

References

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- ▶ Optimal changepoint detection in n data is a non-convex problem, naïvely a $O(n^S)$ computation for S segments.
- ▶ Recent algorithms can compute a globally optimal changepoint model much faster, $O(n \log n)$.
- ▶ Directional constraint graphs specified using domain prior knowledge, or learned using expert labels.
- ▶ Expert labels can also be used as optimization constraints, to ensure that predicted changepoints are consistent.
- ▶ Number of changes can be predicted with new learning algorithms, including ROC curve optimization.
- ▶ Let's collaborate! toby.hocking@nau.edu