Recent advances in supervised optimal changepoint detection

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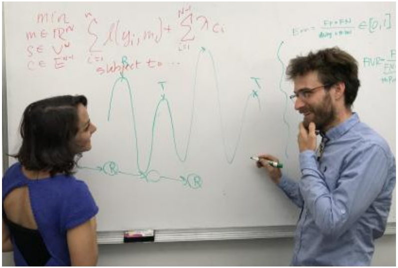
 

Come to Flagstaff!

New algorithms with constraints between adjacent segments

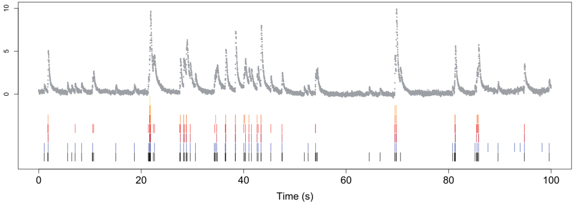
Computing optimal changepoints subject to label constraints

Learning to predict the number of changepoints

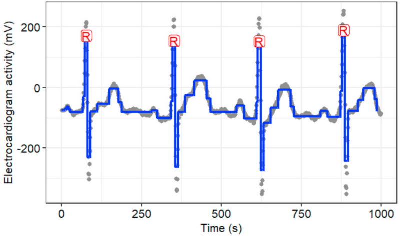
Summary and Discussion

Changepoint detection algorithms for data over time

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

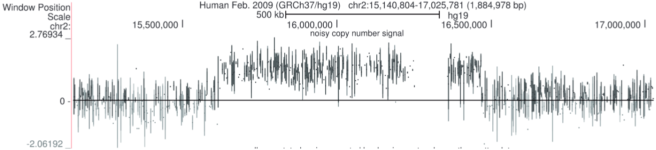


Electrocardiograms (heart monitoring), Fotoohinasab *et al.*, Asilomar conference 2020.

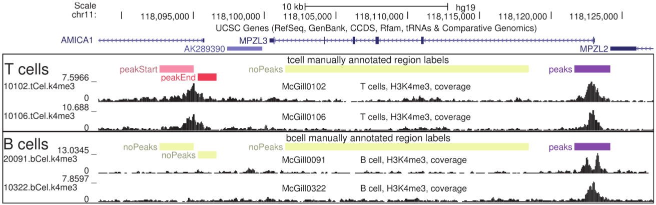


Changepoint detection algorithms for data over space

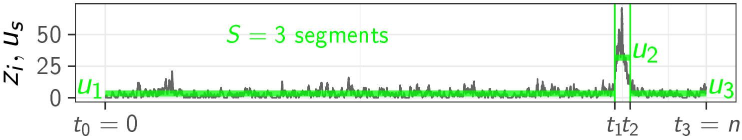
DNA copy number data for cancer diagnosis, Hocking *et al.*, Bioinformatics 2014.



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



Optimal changepoint detection problem and algorithms



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

- Algorithm inputs n data $z_1, \dots, z_n$ and # of segments S.
- Goal is to compute best $S-1$ changepoints $t_1 < \cdots < t_{S-1}$ 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.
- Rigaill 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.

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

$$\text{subject to} \quad u_{s-1} \leq u_s \ \forall s \in \{2,4,\dots\},$$
$$u_{s-1} \geq u_s \ \forall s \in \{3,5,\dots\}.$$

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

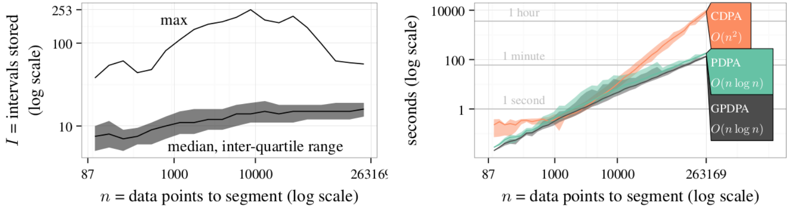
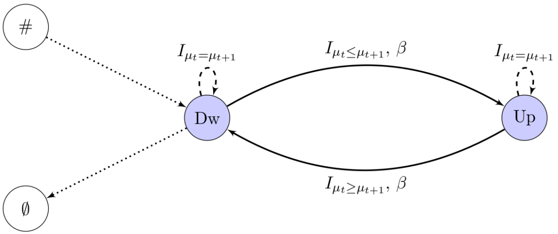
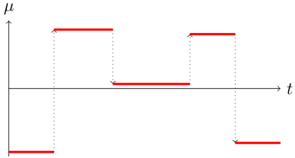


Figure 3: Empirical speed analysis on 2752 count data vectors from the histone mark ChIP-seq benchmark. For each vector we ran the GPDPA with the up-down constraint and a max of $K = 19$ segments. The expected time complexity is $O(KnI)$ where I is the average number of intervals (function pieces; candidate 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

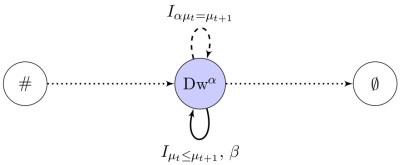
Runge *et al.*, Pre-print arXiv:2002.03646 (graph figures).

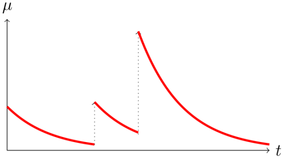




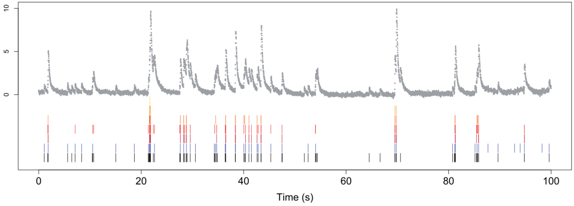
- Purple Dw/Up nodes represent hidden states.
- #/∅ nodes constrain start/end state.
- Edges represent possible state transitions.
- `gfpop` R package with C++ code computes optimal changepoints for user-defined constraint graphs.

All up changes, exponential decaying segments

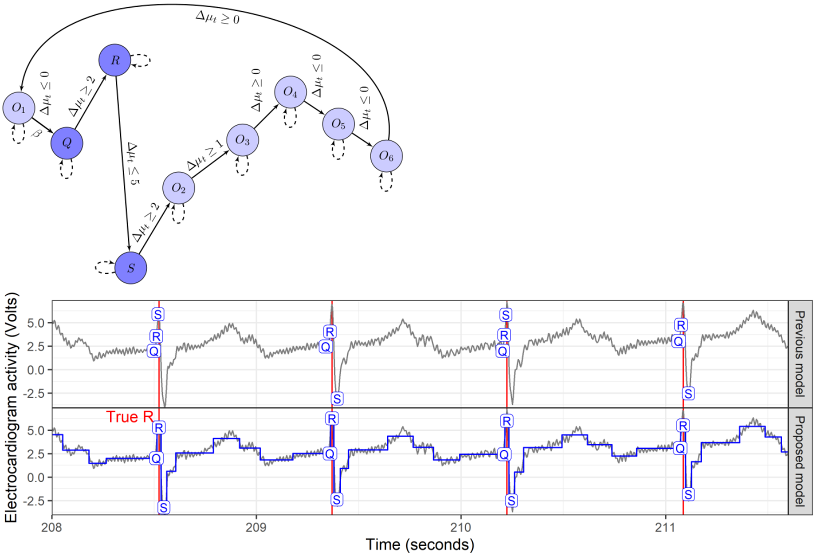




Jewell *et al.*, Biostatistics 2019.



Complex graph for electrocardiogram data



Fotoohinasab *et al.*, Asilomar conference 2020.

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- **Hocking TD**, Boeva V, Rigaill 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.
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- **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):140, 2020.
- Runge V, **Hocking TD**, Romano G, Afghah F, Fearnhead P, Rigaill G. gfpop: an R Package for Univariate Graph-Constrained Change-point Detection. Under review at Journal of Statistical Software. Pre-print arXiv:2002.03646.

New algorithms with constraints between adjacent segments

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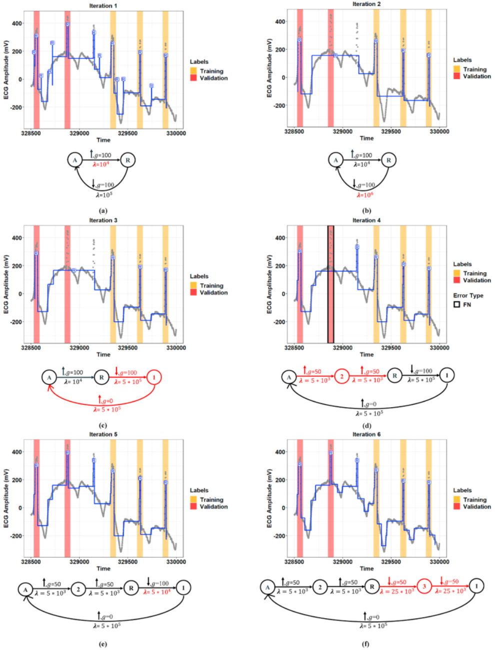
Summary and Discussion

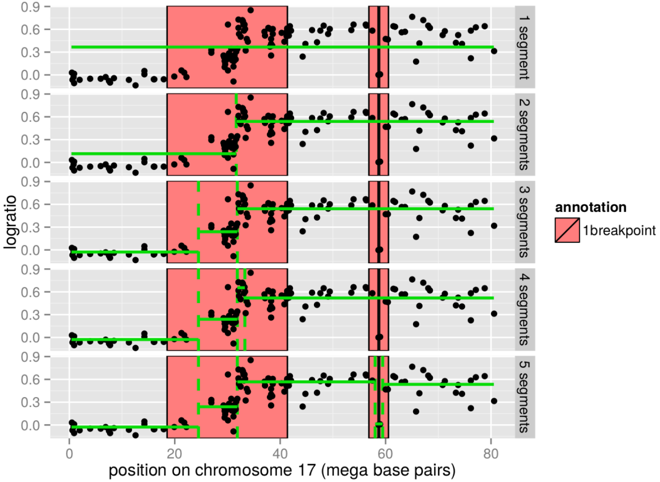
Learning a complex graph using labels



- 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?

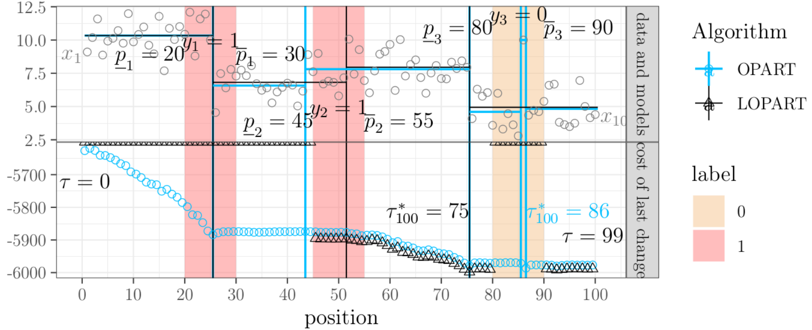
Hocking and Rigaill, Pre-print hal-00759129.



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

Using expert labels as optimization constraints

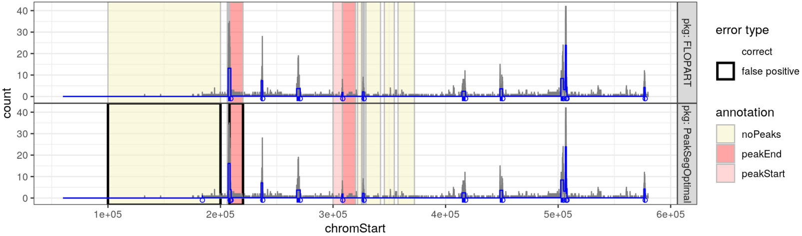
Hocking and Srivastava, Pre-print arXiv:2006.13967.



- Previous OPART model (blue) ignores 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. Under review at Computational Statistics. Pre-print arXiv:2006.13967.
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Summary and Discussion

How to predict the number of changes?

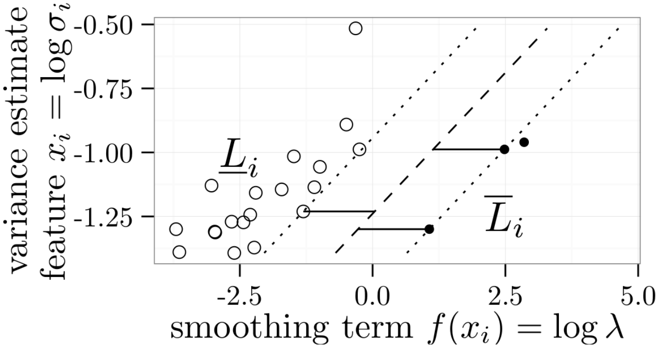
We assumed that the number of segments S is provided as an input parameter to our optimization algorithm.

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

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

Learning to predict number of changes similar to SVM

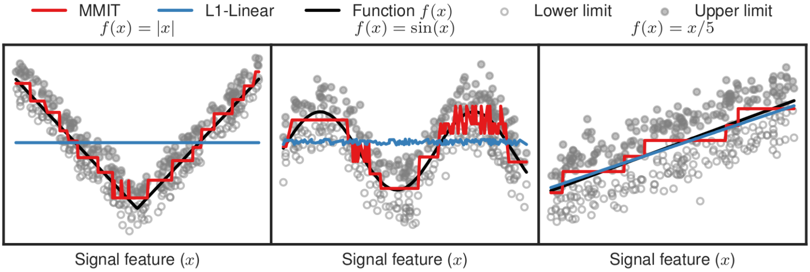
Hocking *et al.*, Int'l Conference on Machine Learning 2013.



- 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

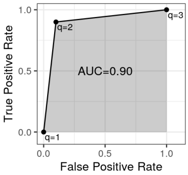
Drouin *et al.*, Neural Information Processing Systems 2017.



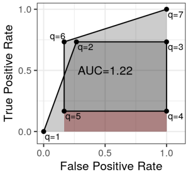
- Generalization of classical CART regression tree learning algorithm.
- Can learn non-linear functions of inputs.
- More recently we implemented a similar idea in xgboost, Barnwal *et al.*, Pre-print arXiv:2006.04920.

Is maximizing Area Under the ROC Curve desirable?

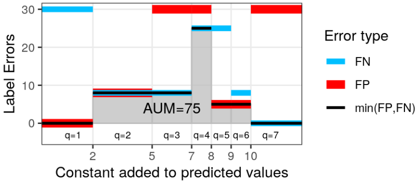
In binary classification the ROC curve is monotonic.



In changepoint detection it can have loops.

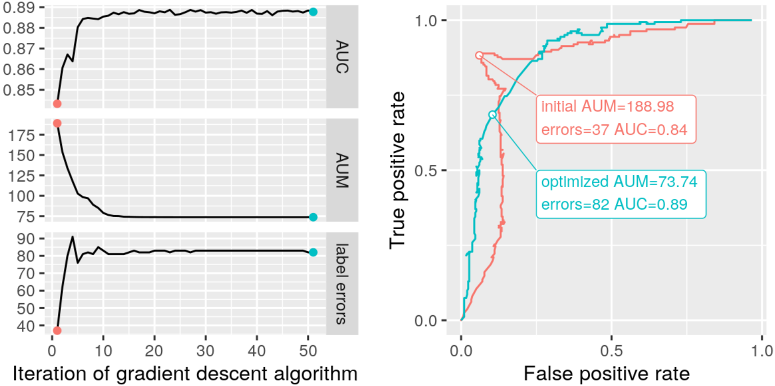


We propose instead to minimize the AUM = Area Under the Minimum of false positives and false negatives, as a function of prediction threshold.



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