# Frontiers in optimal change-point detection algorithms

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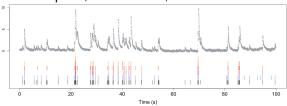


- 1. Introduction, applications, recent algorithms
- 2. Constraints between adjacent segment means
- 3. Optimal changepoints subject to label constraints
- 4. Learning to predict the number of changepoints

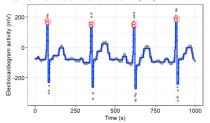
Summary and Discussion

# Changepoint detection algorithms for data over time

Neuron spikes, Jewell et al., Biostatistics 2019.

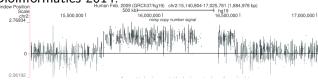


Electrocardiograms (heart monitoring), Fotoohinasab *et al.*, Asilomar conference 2020.

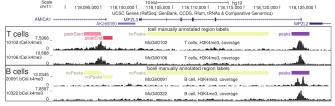


# Changepoint detection algorithms for data over space

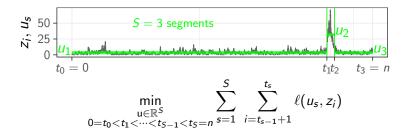
DNA copy number data for cancer diagnosis, Hocking *et al.*, Bioinformatics 2014.



ChIP-seq data for annotating active/inactive regions in different cell types, Hocking *et al.*, Bioinformatics 2017.

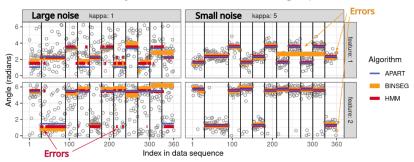


## Optimal changepoint detection problem



- ▶ Algorithm inputs n data  $z_1, ..., z_n$  and # of segments S.
- ▶ Loss function  $\ell$  measures fit of means  $u_s$  to data  $z_i$ .
- ▶ Goal is to compute best S-1 changepoints  $t_1 < \cdots < t_{S-1}$  and S segment parameters  $u_1, \ldots, u_S$ .
- Non-convex optimization problem, naïvely  $O(n^S)$  time.
- ► Fast approximate heuristic algorithms?

### Fast heuristics can yield inaccurate change-points



- ► Simulation: angular data, 2 dimensions/features.
- Heuristics are approximate optimization algorithms.
- Fast: linear O(n) time for n data.
- ▶ Not guaranteed to compute change-points with best loss.
- ▶ BINSEG = Binary segmentation (Scott and Knott, 1974).
- HMM = Hidden Markov Model (Rabiner, 1989).



## Constrained problem, Lasso heuristic

#### **Constrained** optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \sum_{i=1}^n \ell(\mu_i, z_i) \quad \text{subject to} \qquad \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i] \leq S.$$
 Number of change-points (regularization)

- Hyper-parameter is number of segments S.
- ▶ Indicator function  $I[\cdot] \in \{0,1\}$  is non-convex.
- Gradient descent yields local min.
- Analog with best subset regression: hyper-parameter is number of variables (combinatorial search, relax to Lasso).
- ▶ Fused Lasso for change-points (Tibshirani et al., JRSSB 2005).
- Lasso selects too many variables (false positive change-points).

# Constrained problem, classic dynamic programming solution

Constrained optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \sum_{i=1}^n \ell(\mu_i, z_i) \quad \text{subject to} \quad \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i] \leq S.$$
 Number of change-points (regularization)

- Auger and Lawrence, Algorithms for the optimal identification of segment neighborhoods, Bull Math Biol (1989).
- Optimal recursive updates (dynamic programming algorithm).
- ▶ Let  $C_{n,S}$  be best cost up to n data and S segments.
- ▶ Start by computing  $C_{1,1}$  to  $C_{1,n}$  (cum sum).
- ▶ Then compute  $C_{2,2}$  to  $C_{2,n}$ ,  $C_{3,3}$ , ...,  $C_{3,n}$ , etc.
- Output all optimal models from 1 to S segments.
- ▶ Time complexity  $O(Sn^2)$  faster than naïve  $O(n^S)$ .
- Still too slow for large data n and model sizes S.



# Penalized problem, classic dynamic programming solution

Penalized optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \sum_{i=1}^n \ell(\mu_i, z_i) \ + \qquad \underbrace{\lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i]}_{\text{Loss (data-fitting)}} \ + \qquad \underbrace{\lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i]}_{\text{Number of change-points (regularization)}}$$

- Hyper-parameter is non-negative penalty  $\lambda \geq 0$ .
- ▶ Jackson, et al., An algorithm for **optimal partitioning** of data on an interval, IEEE Sig Proc Lett (2005).
- Optimal recursive updates (dynamic programming algorithm).
- Let  $C_n$  be best cost up to n data.
- ▶ Recursively compute  $C_1, C_2, \ldots, C_n$ .
- ▶ Time complexity  $O(n^2)$  faster than  $O(Sn^2)$ .
- User can not directly specify number of segments S.
- $\triangleright$  Output one optimal change-point model (not all in  $1, \ldots, S$ ).
- ► Quadratic time is still too slow for large data n.

## Penalized problem, PELT algorithm

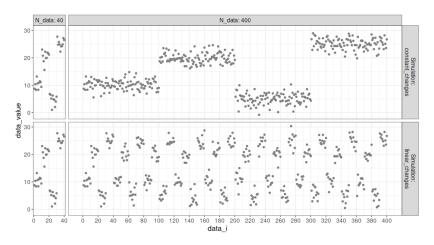
Penalized optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \sum_{i=1}^n \ell(\mu_i, z_i) \ + \qquad \lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i].$$
 Loss (data-fitting) Number of change-points (regularization)

- ▶ Recursively compute  $C_1, C_2, \ldots, C_n$ .
- Classic DP considers all previous change-points.
- At time n, consider  $C_1, \ldots, C_{n-1}$ .
- Pruned Exact Linear Time algo: Killick, et al., JASA (2012).
- ▶ At time *n* consider only a subset of  $C_1, ..., C_{n-1}$ .
- ► Easy to implement, with only 1 additional line of code!
- Same output: one optimal change-point model.
- ▶ Time complexity: best O(n), worst  $O(n^2)$ .



## Simulated data with constant and linear changes

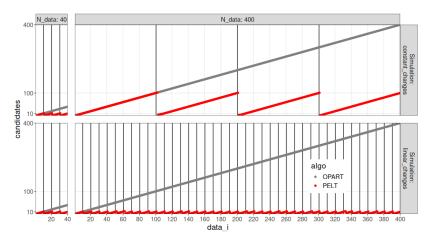


- ightharpoonup Constant changes: always 4 segments (for any data size n).
- Linear: change every 10 data.

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



## PELT algorithm demonstration



- After each change in data, PELT prunes prior candidates.
- ► More changes—more pruning—faster.

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



## Penalized problem, PELT algorithm

**Penalized** optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \sum_{i=1}^n \ell(\mu_i, z_i) \ + \qquad \lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i].$$
 Loss (data-fitting) Number of change-points (regularization)

# changes in data	Algorithm	# candidates per data	Overall time
Constant $O(1)$	OPART	O(n)	$O(n^2)$
	PELT	O(n)	$O(n^2)$
Linear $O(n)$	OPART	O(n)	$O(n^2)$
	PELT	O(1)	O(n)

- ▶ PELT fast/linear for data with frequent changes.
- ▶ But slow/quadratic for long runs of data without changes.
- ► Can we go faster when there are no changes?

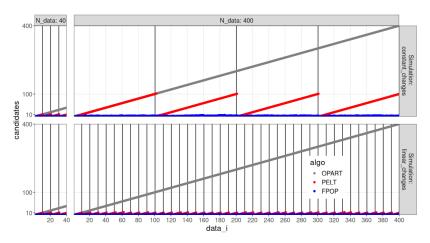
## Yes, faster with FPOP algorithm!

#### Penalized optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \underbrace{\sum_{i=1}^n \ell(\mu_i, z_i)}_{\text{Loss (data-fitting)}} \ + \ \underbrace{\lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i]}_{\text{Number of change-points (regularization)}}$$

- ► FPOP algo: Maidstone, et al., Stat. and Comp. (2017).
- Let  $C_n(m)$  be the best cost with mean m at n data.
- ▶ Recursively compute functions  $C_1(m)$ ,  $C_2(m)$ , ...,  $C_n(m)$ .
- ► Functional pruning considers a small subset of candidates.
- Same output: one optimal change-point model.
- ▶ Same time as PELT in theory: best O(n), worst  $O(n^2)$ .
- ▶ But much faster in practice!

#### FPOP algorithm demonstration



► FPOP always prunes, whether or not there are changes in data. https://tdhock.github.io/blog/2025/PELT-vs-fpopw/

## Penalized problem, FPOP algorithm

**Penalized** optimal change-point problem:

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	FPOP	$O(\log n)$	$O(n \log n)$
Linear $O(n)$	OPART	O(n)	$O(n^2)$
	PELT	O(1)	O(n)
	FPOP	O(1)	O(n)

- ▶ FPOP always fast in 1d data, no matter how many changes.
- ▶ Worst case  $O(n^2)$  only happens in pathological data.



## Penalized problem, FPOP algorithm

#### Penalized optimal change-point problem:

$$\min_{\mu \in \mathbb{R}^n} \ \underbrace{\sum_{i=1}^n \ell(\mu_i, z_i)}_{\text{Loss (data-fitting)}} + \underbrace{\lambda \sum_{i=2}^n I[\mu_{i-1} \neq \mu_i]}_{\text{Number of change-points (regularization)}}$$

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- Functional pruning considers a small subset of candidates.
- Same output: one optimal change-point model.
- ▶ Time complexity best O(n), worst  $O(n^2)$ .

## Penalized problem, FPOP extensions

#### Functional pruning can handle:

- ▶ Inequality constraints between segment means (next section).
- Robust loss functions: Fearnhead and Rigaill, JASA (2019).
- Auto-regressive models: Romano et al., JASA (2021).
- Storage on disk: Hocking et al., JSS (2022).
- Multi-variate time series: Pishchagina et al., Computo (2024).
- Multi-scale penalties: Liehrmann and Rigaill, JCGS (2025).

#### But:

- Difficult to implement (100s of lines of C++ code).
- Not as fast in high dimensional data/models.

Is it possible to go faster?

## Yes, faster with DUST algorithm!

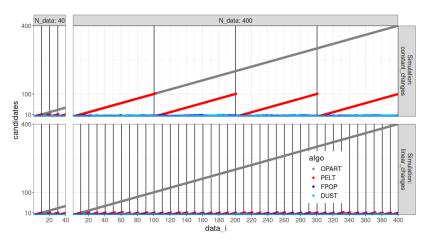
Penalized optimal change-point problem:

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- Truong and Runge, An Efficient Algorithm for Exact Segmentation of Large Compositional and Categorical Time Series, Stat (2024).
- DUST algo: DUality Sample Test.
- Combines ideas from PELT and FPOP algos.
- Solve a Langrange dual problem to prune change-points.
- Easier to code than FPOP.
- ▶ Same time as PELT/FPOP in theory: best O(n), worst  $O(n^2)$ .
- But much faster in practice!

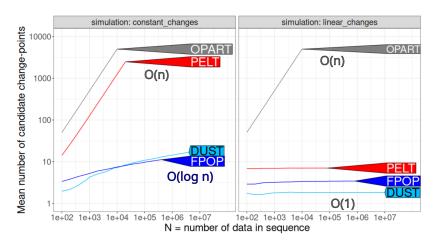


#### DUST algorithm demonstration



▶ DUST always prunes, whether or not there are changes in data. https://tdhock.github.io/blog/2025/PELT-vs-fpopw/

#### Number of candidates considered

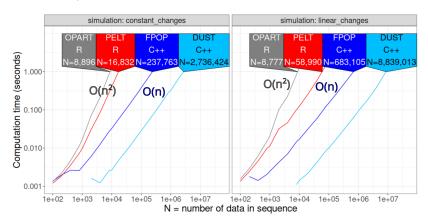


- ▶ Data sizes varied from 100 to 10,000,000.
- Slope on log-log plot indicates asymptotic time complexity.

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



#### Overall computation time



- N= data size computable in time limit of 1 second.
- FPOP 10x faster than PELT.
- ▶ DUST 10x faster than FPOP.

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



#### Penalized problem, DUST algorithm

Penalized optimal change-point problem:

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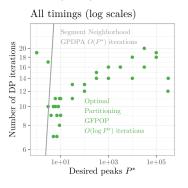


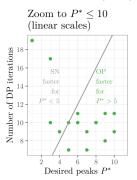
## Computing various solutions using penalized solver

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  $\lambda$  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:  $\lambda \in [0.1, \overline{1}0.5]$ ?
- 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).

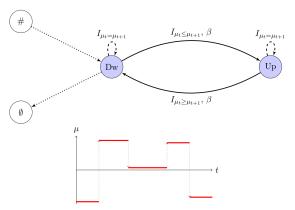
If M is the number of models to compute (ex: 11 models from 50 to 60 change-points), then  $O(M + \log \overline{P})$  DP iterations—fast for large model sizes  $\overline{P}$ .

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Summary and Discussion

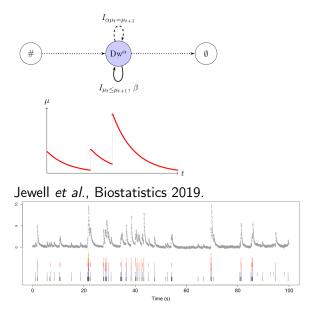
# Optimization constraints defined using a graph

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

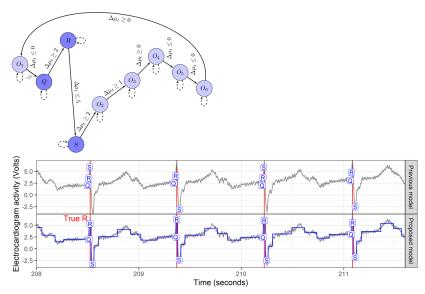


- Purple Dw/Up nodes represent hidden states.
- ► #/Ø nodes constrain start/end state.
- Edges represent possible state transitions.
- gfpop R package with C++ code computes optimal changepoints for user-defined constraint graphs.

## All up changes, exponential decaying segments



# Complex graph for electrocardiogram data



Fotoohinasab et al., Asilomar conference 2020.

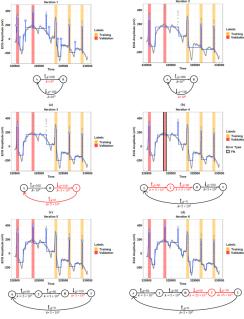


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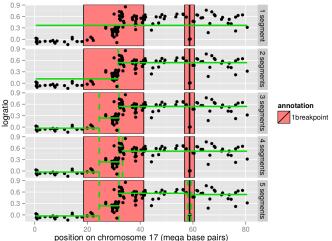
# Learning a complex graph using labels



- 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 Rigaill, Pre-print hal-00759129.

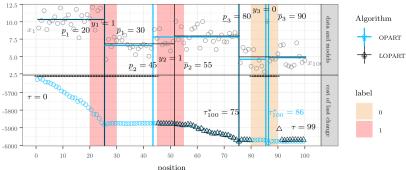


- Expert wants: one changepoint in each label (red rectangle).
- ▶ No model is consistent with all three labels.



## Using expert labels as optimization constraints

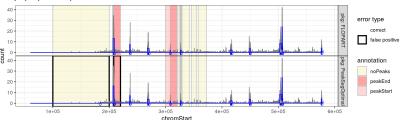
Hocking and Srivastava, Computational Statistics 38 (2023).



- 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

Kaufman et al., Journal of Computational and Graphical Statistics 33(4) (2024).



- 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.

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Summary and Discussion

### How to predict the number of changes?

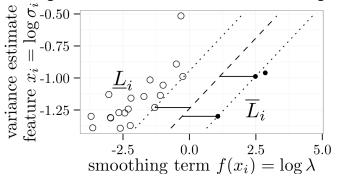
We assumed that the number of segments S is provided as an input parameter to our optimization algorithm.

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

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

## Learning to predict number of changes similar to SVM

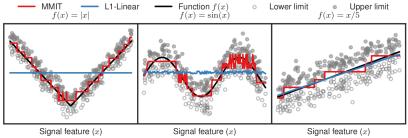
Hocking et al., Int'l Conference on Machine Learning 2013.



- ► 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.

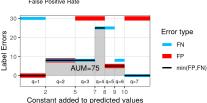
AUC=0.90

AUC=0.90

False Positive Rate

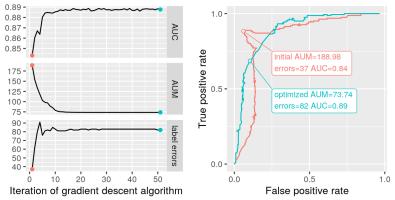
In changepoint detection it can have loops.

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.

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## Summary and Discussion

- Poptimal 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

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