Labeled Optimal Partitioning

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August 31, 2020

Introduction: supervised changepoint detection for cancer diagnosis with DNA copy number data

Labeled Optimal Partitioning (LOPART)

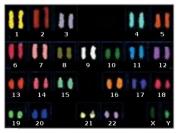
LOPART Demo

Results and Discussion

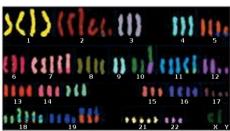
Cancer cells show chromosomal copy number alterations

Spectral karyotypes show the number of copies of the sex chromosomes (X,Y) and autosomes (1-22).

Source: Alberts *et al.* 2002.

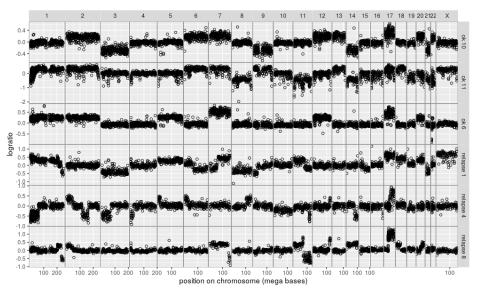


Normal cell with 2 copies of each autosome.

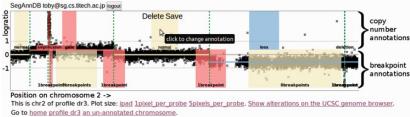


Cancer cell with many copy number alterations.

DNA copy number profiles from neuroblastoma patients with or without relapse



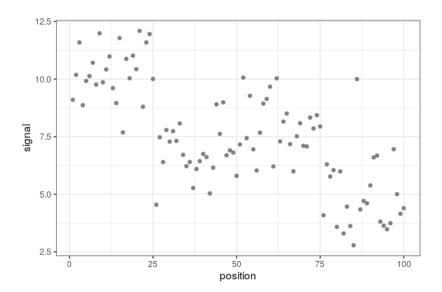
Previous work: SegAnnDB interactive machine learning system



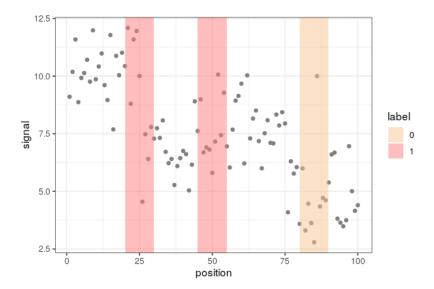
Hocking et al., 2014.

- User uploads noisy data sets for machine learning analysis.
- ▶ User can provide labels which indicate presence(1) or absence(0) of changepoints in specific regions of data sets.
- Classic optimal changepoint model (max penalized Gaussian likelihood) used if it has zero label errors. OPART algorithm, Jackson et al., 2005. FPOP algorithm, Maidstone et al., 2016.
- ► Label-aware SegAnnot algorithm used otherwise (Hocking and Rigaill, 2012). Always zero train label errors, but never predicts any changepoints outside of positive(1) labels.

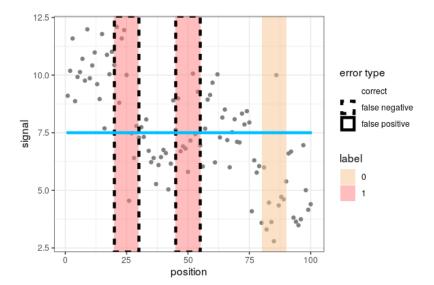
Example noisy data sequence



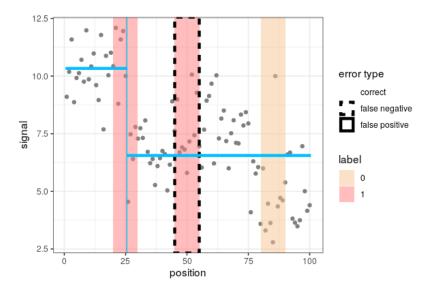
Example noisy data sequence with labels



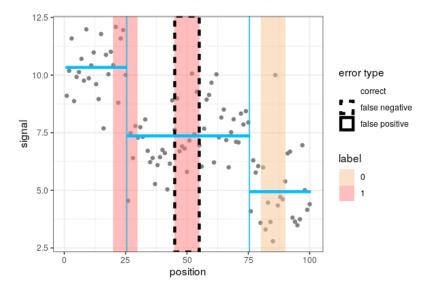
OPART with penalty $\lambda = 1000$ (ignores labels)



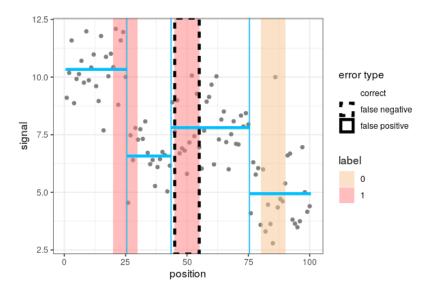
OPART with penalty $\lambda = 100$ (ignores labels)



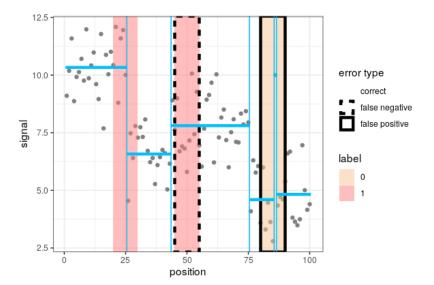
OPART with penalty $\lambda = 20$ (ignores labels)



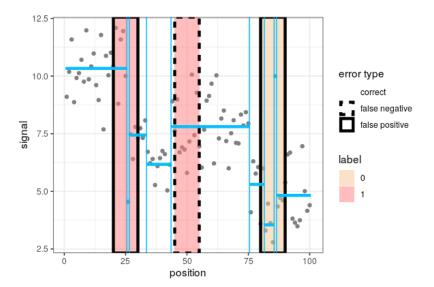
OPART with penalty $\lambda = 15$ (ignores labels)



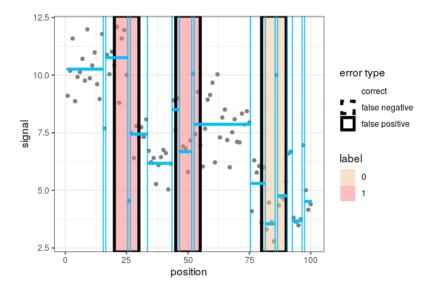
OPART with penalty $\lambda = 10$ (ignores labels)



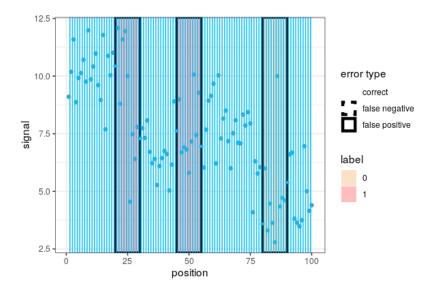
OPART with penalty $\lambda = 5$ (ignores labels)



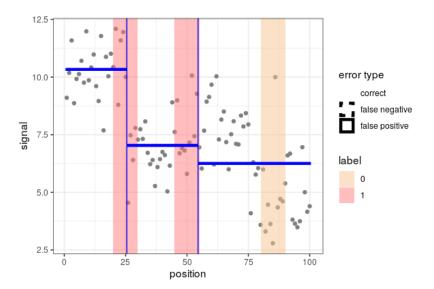
OPART with penalty $\lambda = 4$ (ignores labels)



OPART with penalty $\lambda = 0$ (ignores labels)



SegAnnot (no changes in unlabeled regions)



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Baseline/previous OPART algorithm

Assume

- ▶ $\mathbf{x} = [x_1 \cdots x_N]$ is the sequence of N data,
- \blacktriangleright ℓ is a loss function (e.g. square loss),
- ▶ *I* the indicator function counts the number of changes,
- \triangleright λ is a non-negative penalty (larger for fewer changes).

Then the problem and algorithm are

$$\hat{C}_{N} = \min_{\mathbf{m} \in \mathbb{R}^{N}} \sum_{i=1}^{N} \ell(m_{i}, x_{i}) + \lambda \sum_{i=1}^{N-1} I[m_{i} \neq m_{i+1}].$$

$$= \min_{\tau \in \{0, 1, ..., N-1\}} \hat{C}_{\tau} + \lambda + L(\tau + 1, N, \mathbf{x}).$$

where

- ightharpoonup au is the last changepoint optimization variable,
- $ightharpoonup \hat{C}_{ au}$ is the optimal cost computed in previous iteration au,
- L is the cost of the last segment.

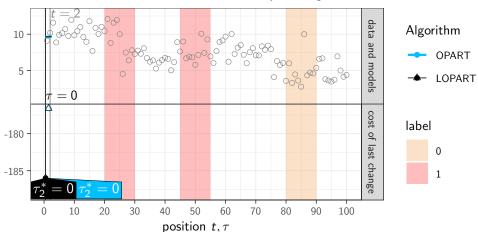


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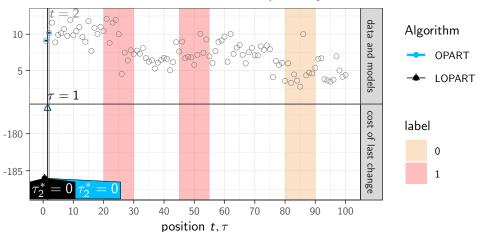
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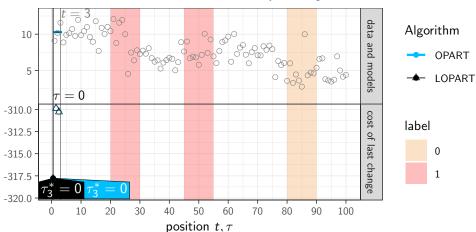
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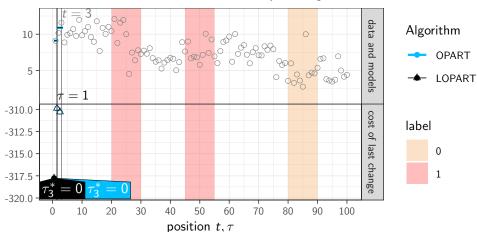
$$W_t = \min_{ au \in T_t} \underbrace{W_{ au}}_{ ext{optimal cost up to } au} + \underbrace{\lambda}_{ ext{penalty}} + \underbrace{L(au+1,t,\mathbf{x})}_{ ext{optimal cost of last segment}}$$



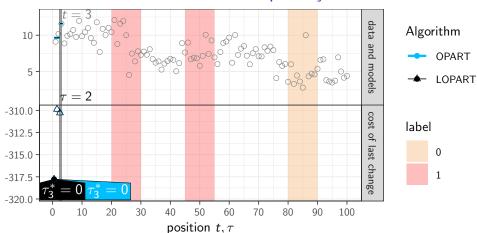
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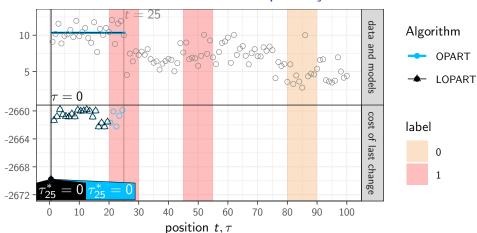
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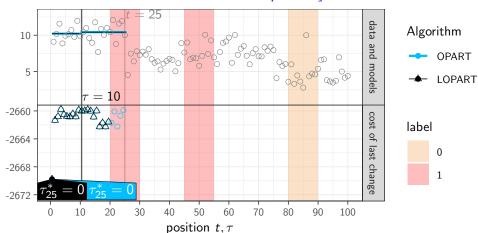
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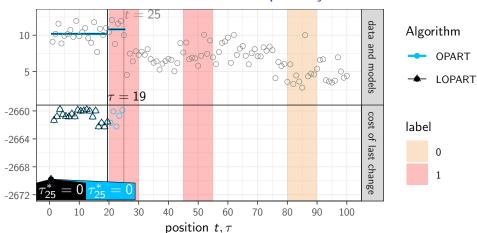
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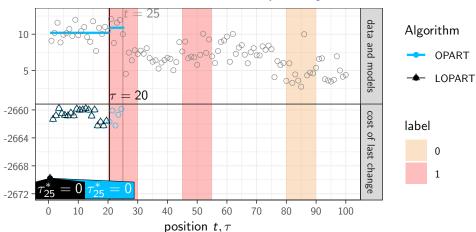
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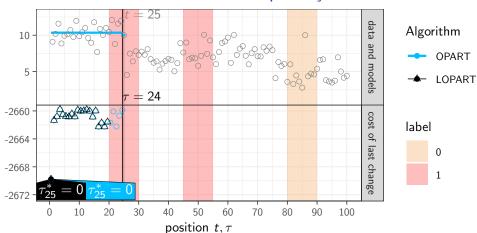
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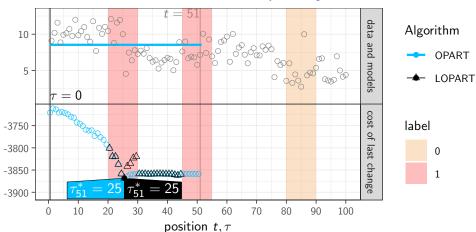
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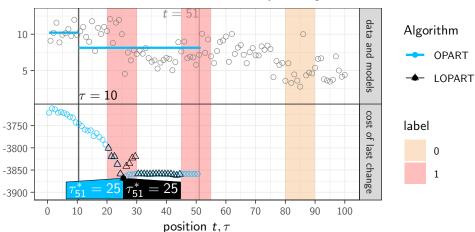
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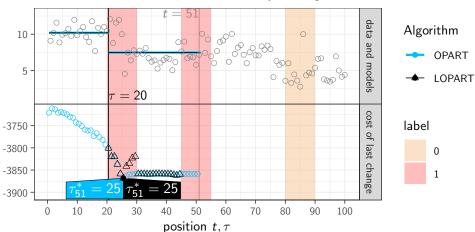
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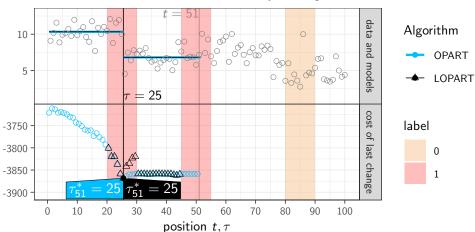
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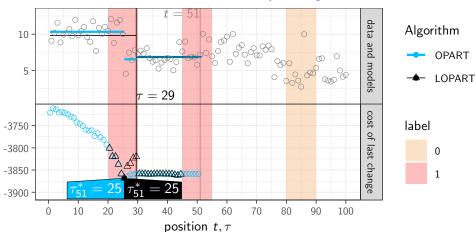
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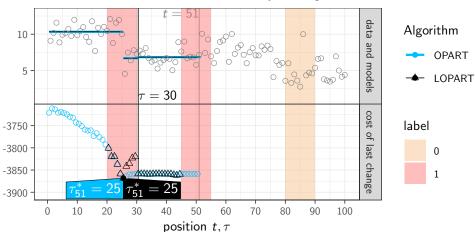
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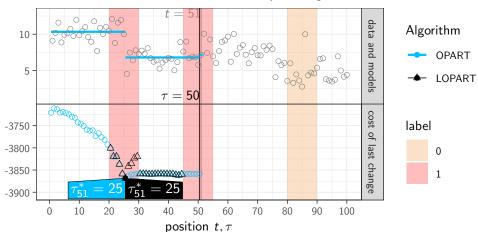
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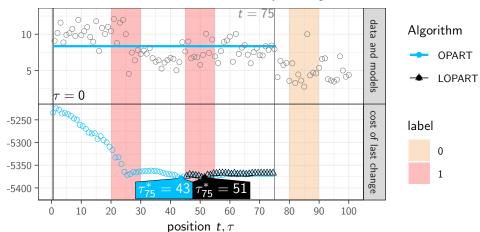
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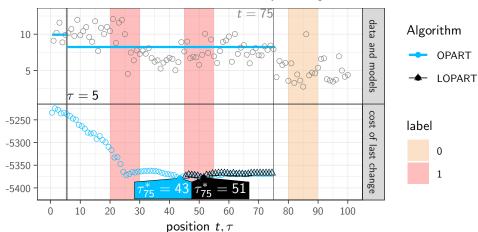
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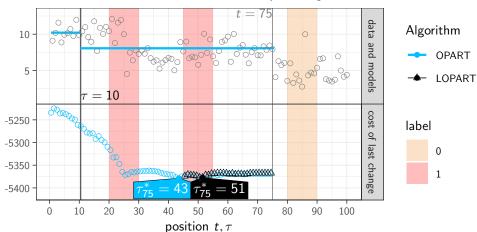
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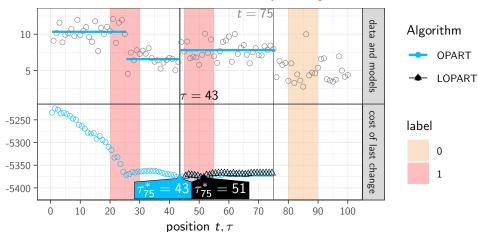
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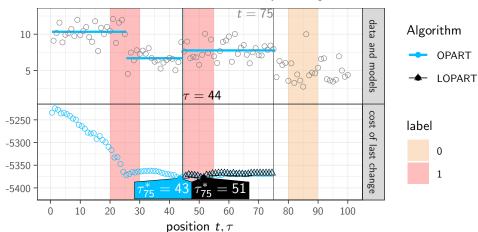
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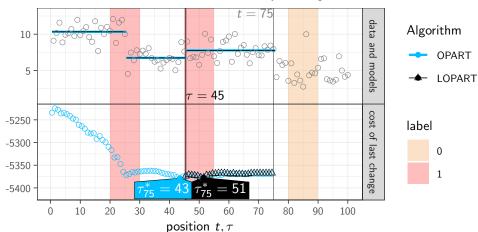
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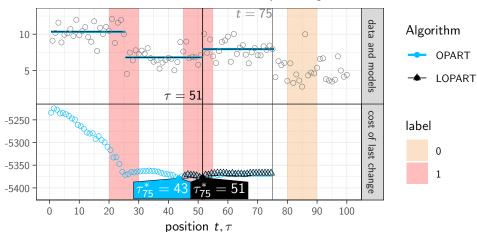
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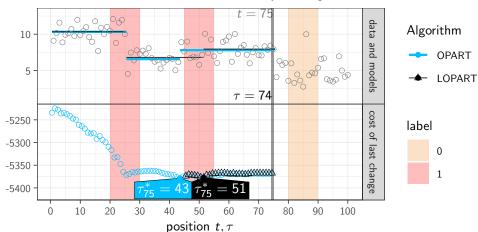
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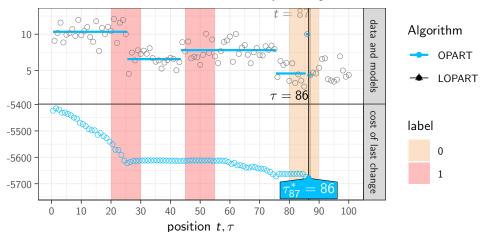
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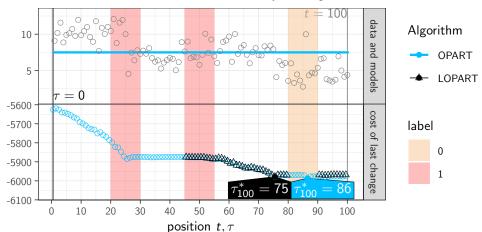
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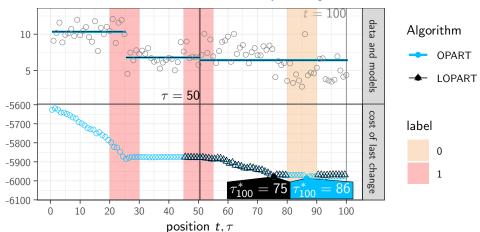
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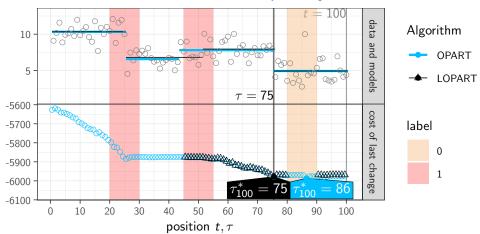
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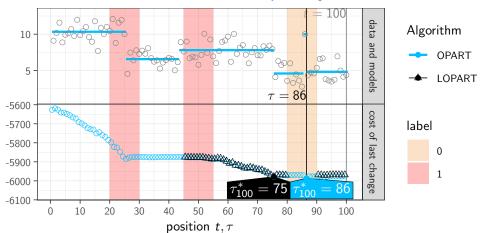
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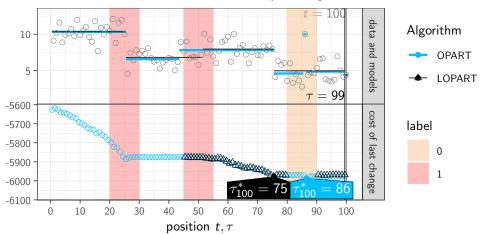
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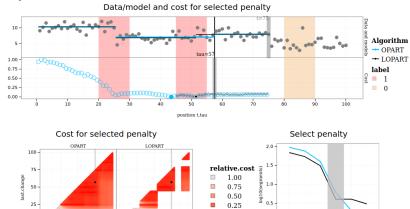
Interactive version

Try this at home:

25 50

100 0 25 50 75 100

up.to.t



0.00

0.0

ó

log10(penalty)

http://members.cbio.mines-paristech.fr/~thocking/figure-candidates-interactive/

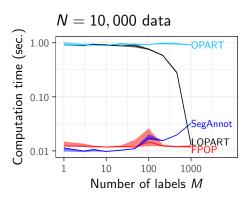
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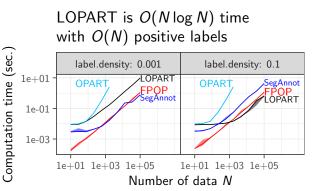
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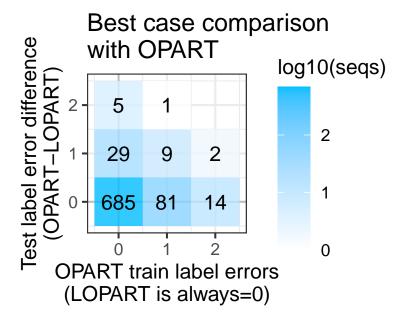
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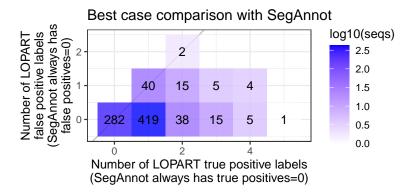
Empirical time complexity (labels)



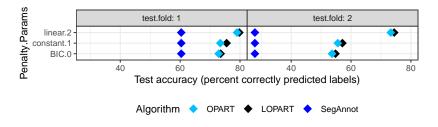
Empirical time complexity (data)



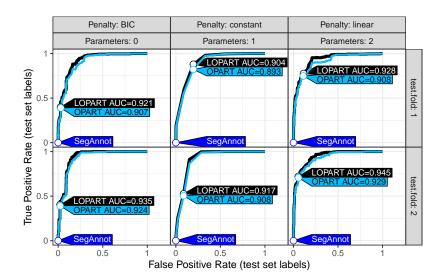




Test accuracy in cross-validation experiments



Test ROC curves in cross-validation experiments



Summary and Discussion

- Proposed algo fixes issues with two previous algorithms (better train AND test accuracy).
- Results demonstrate improved speed and accuracy.
- R package on CRAN and https://github.com/tdhock/LOPART
- Figure/slide code on https://github.com/tdhock/LOPART-paper
- Future work: functional pruning algorithm, which can solve more complex constrained changepoint problems (e.g. change must be non-decreasing), and should be faster (log-linear instead of quadratic).