#### 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)

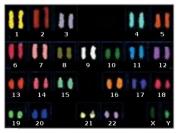
LOPART Demo

Results and Discussion

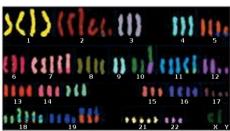
#### Cancer cells show chromosomal copy number alterations

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

Source: Alberts *et al.* 2002.

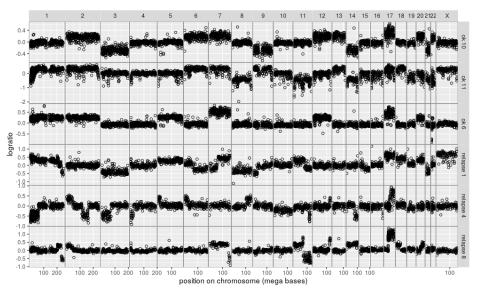


Normal cell with 2 copies of each autosome.

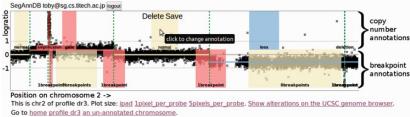


Cancer cell with many copy number alterations.

# DNA copy number profiles from neuroblastoma patients with or without relapse



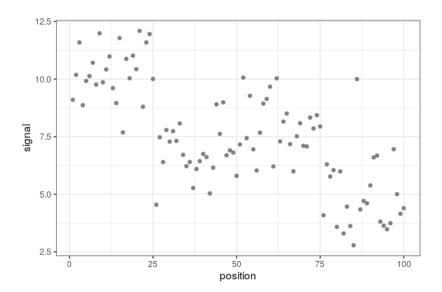
## Previous work: SegAnnDB interactive machine learning system



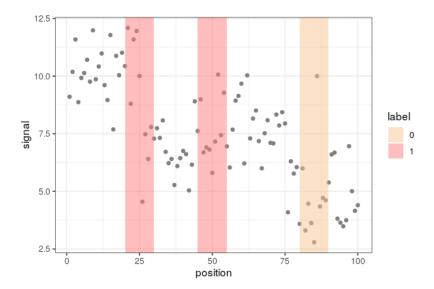
#### Hocking et al., 2014.

- 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.

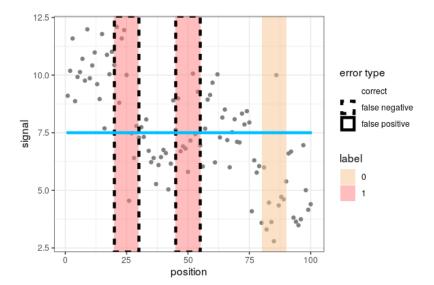
#### Example noisy data sequence



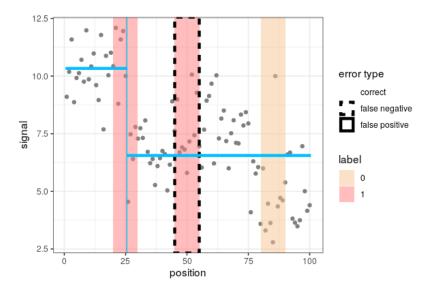
#### Example noisy data sequence with labels



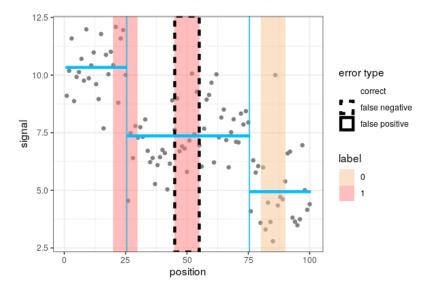
### OPART with penalty $\lambda = 1000$ (ignores labels)



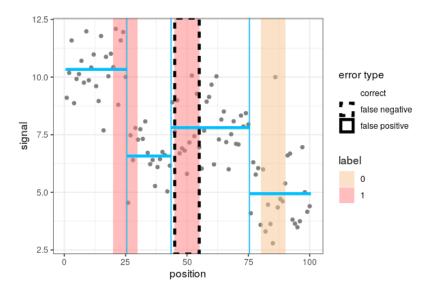
#### OPART with penalty $\lambda = 100$ (ignores labels)



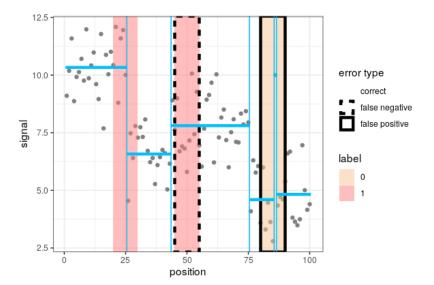
#### OPART with penalty $\lambda = 20$ (ignores labels)



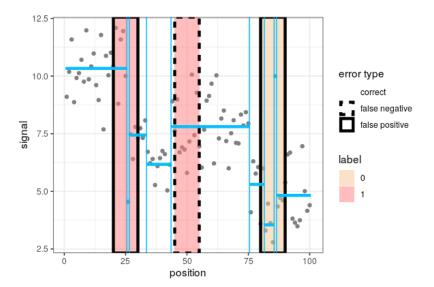
### OPART with penalty $\lambda = 15$ (ignores labels)



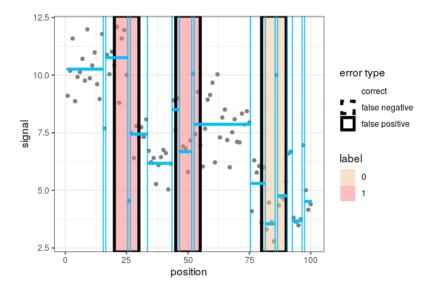
#### OPART with penalty $\lambda = 10$ (ignores labels)



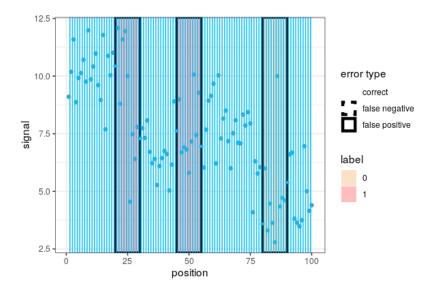
## OPART with penalty $\lambda = 5$ (ignores labels)



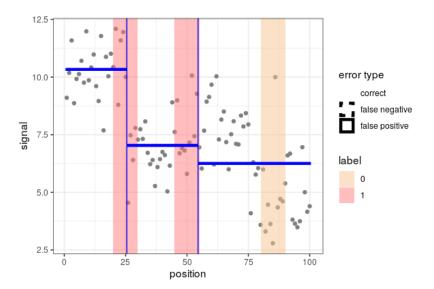
### OPART with penalty $\lambda = 4$ (ignores labels)



### 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,
- $\blacktriangleright$   $\ell$  is a loss function (e.g. square loss),
- ▶ *I* the indicator function counts the number of changes,
- $\triangleright$   $\lambda$  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.

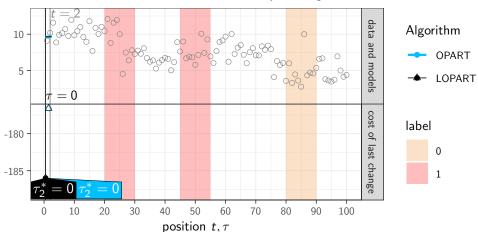


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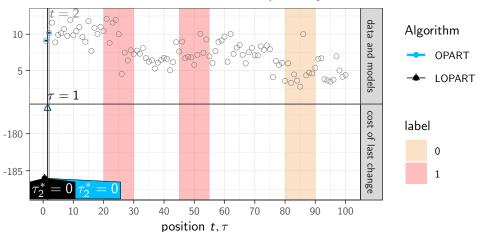
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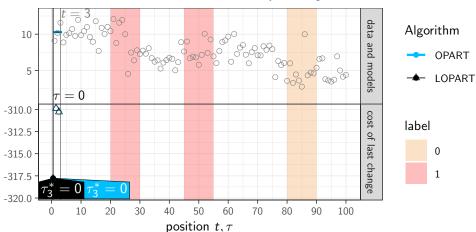
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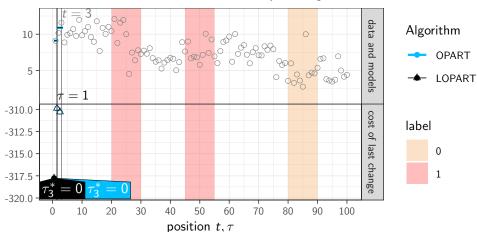
$$W_t = \min_{ au \in T_t} \underbrace{W_{ au}}_{ ext{optimal cost up to } au} + \underbrace{\lambda}_{ ext{penalty}} + \underbrace{L( au+1,t,\mathbf{x})}_{ ext{optimal cost of last segment}}$$



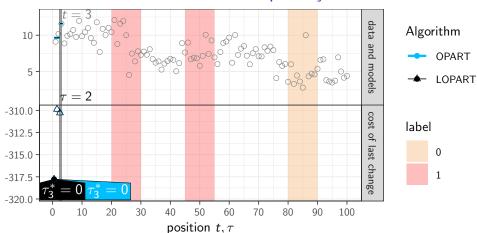
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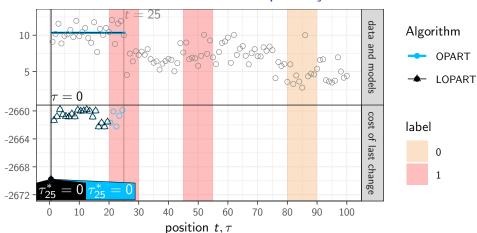
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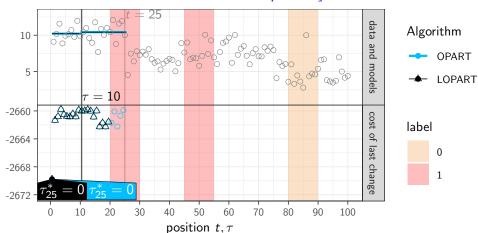
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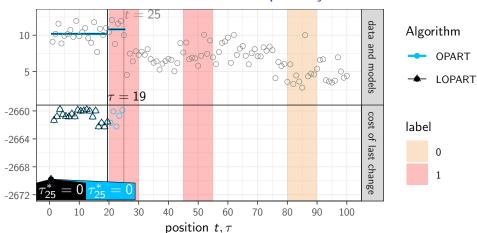
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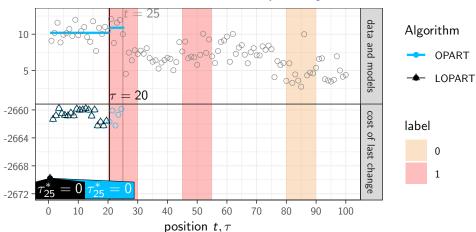
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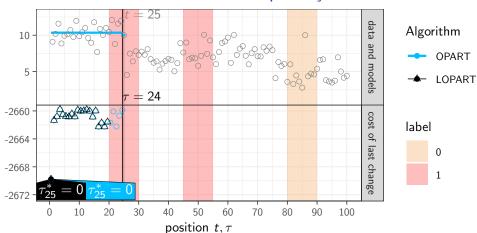
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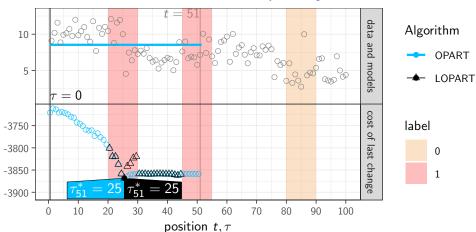
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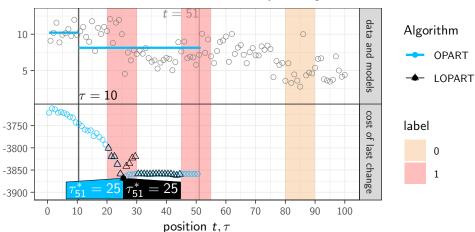
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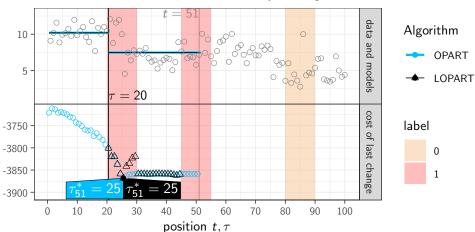
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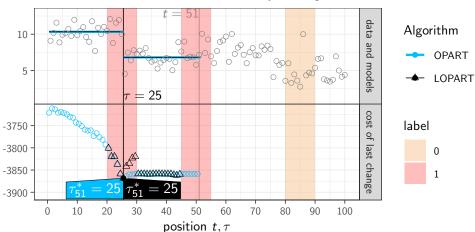
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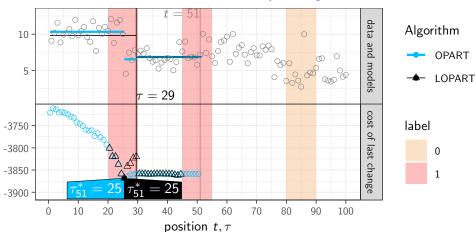
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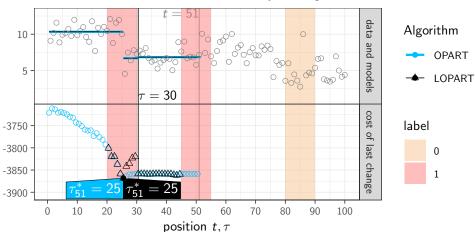
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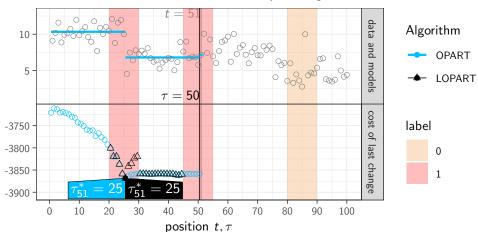
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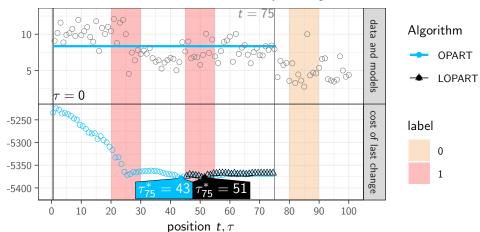
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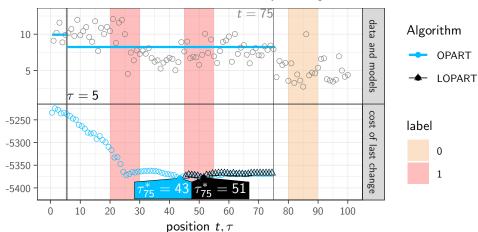
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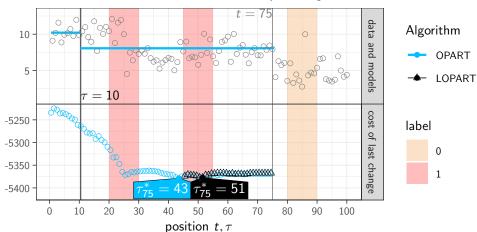
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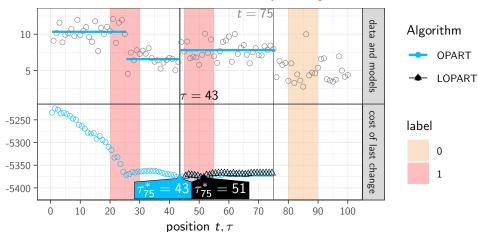
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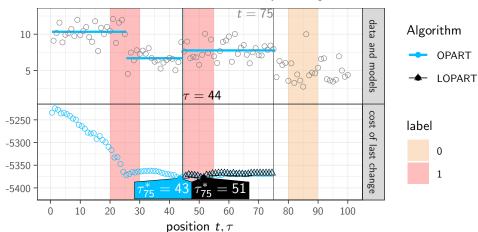
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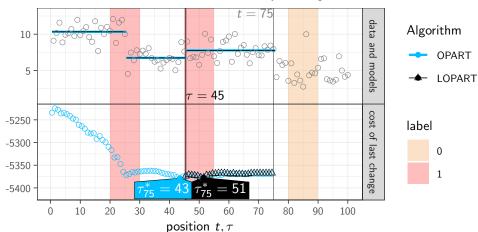
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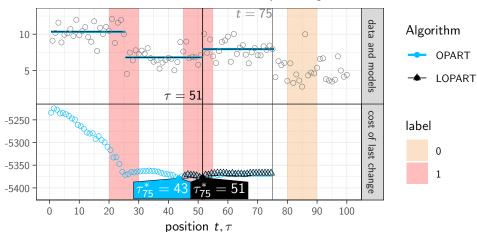
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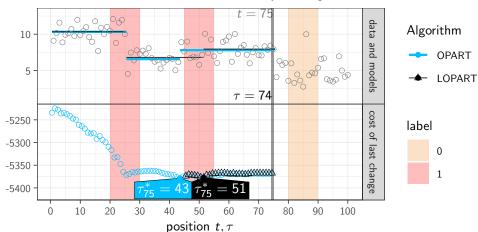
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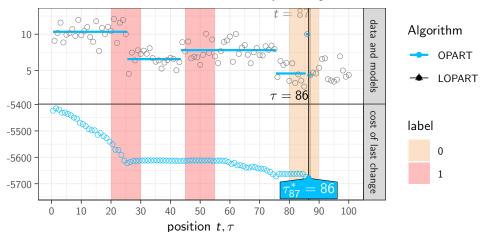
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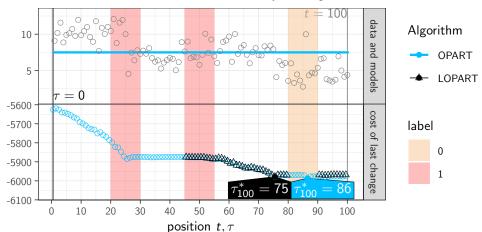
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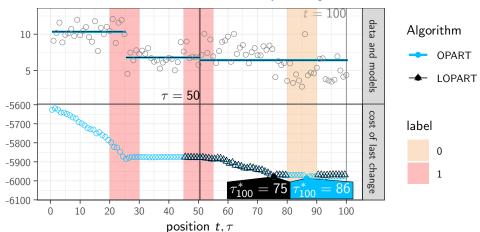
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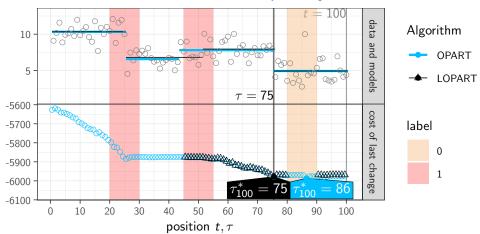
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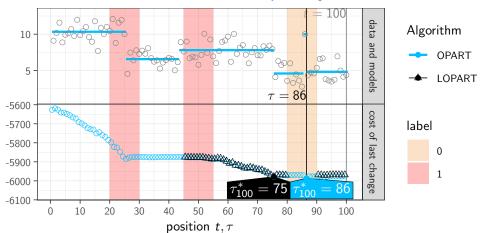
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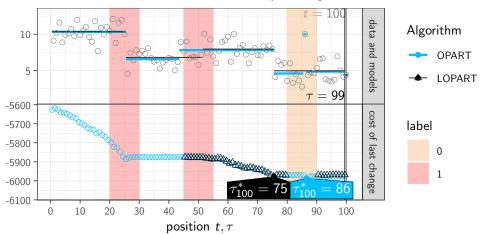
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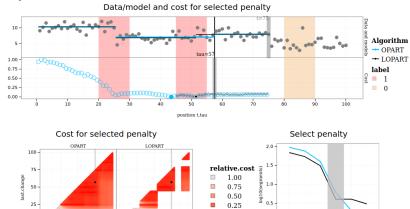
#### Interactive version

#### 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/

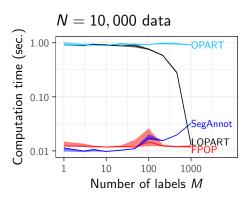
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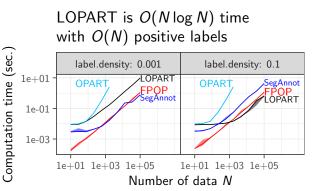
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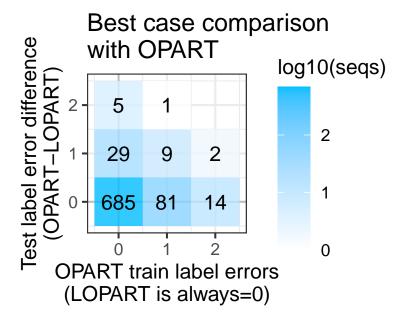
Results and Discussion

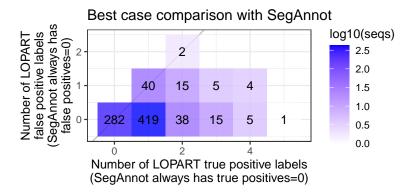
#### Empirical time complexity (labels)



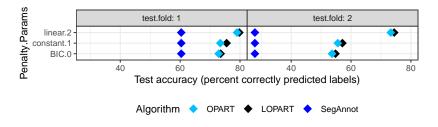
# Empirical time complexity (data)



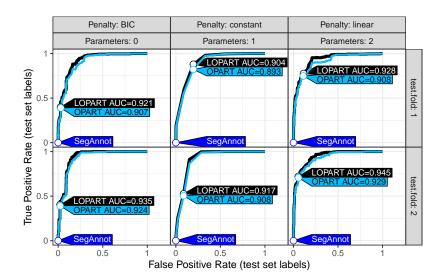




#### Test accuracy in cross-validation experiments



# 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).