Optimal segmentation

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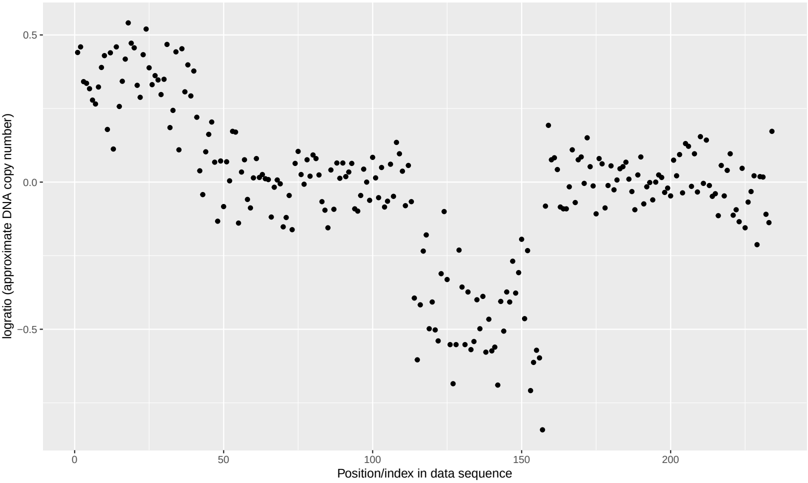
Background: detecting abrupt changes is important

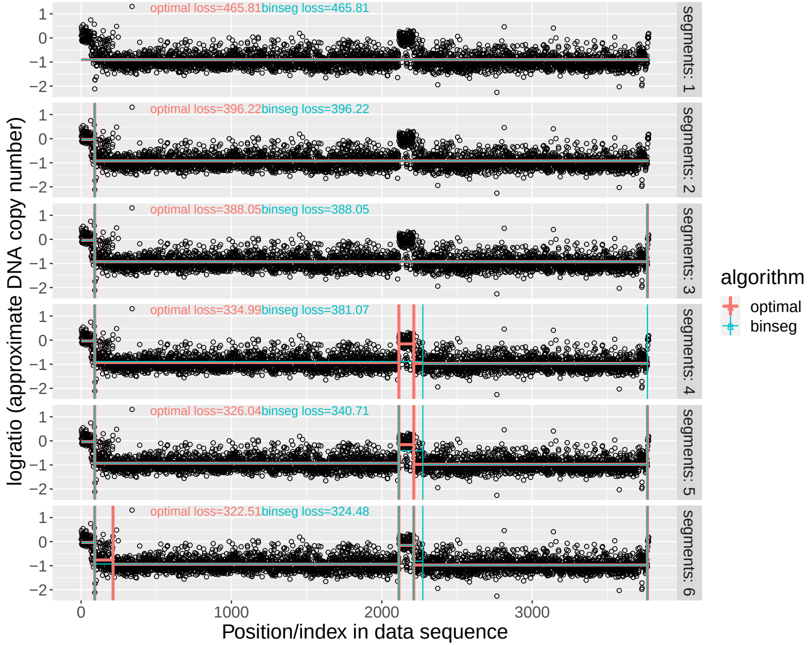
Example from cancer diagnosis: breakpoints are associated with aggressive disease in neuroblastoma.



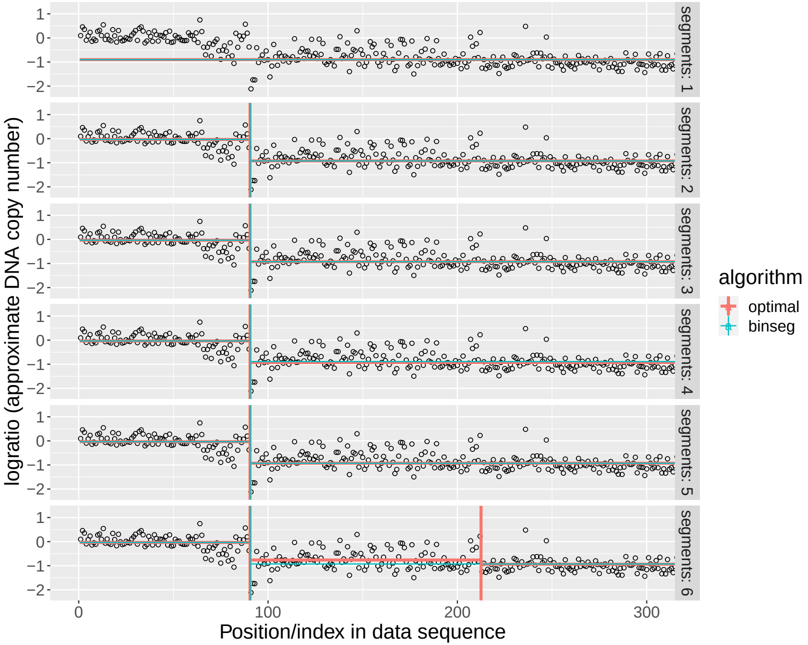
Motivation for optimal detection

- Binary segmentation is a greedy algorithm, so sometimes it chooses a changepoint which is sub-optimal for a larger model size.
- Is it possible to compute the changepoints and segments which are optimal for each model size? Yes, with dynamic programming.
- Dynamic programming can be applied to any computational problem which involves optimization, and can be broken down into independent sub-problems. In this context we use it to compute the changepoints and segments which are optimal for a given loss function.
- Is it desirable to compute the optimal changepoints and segments? Yes, see examples in next slides.

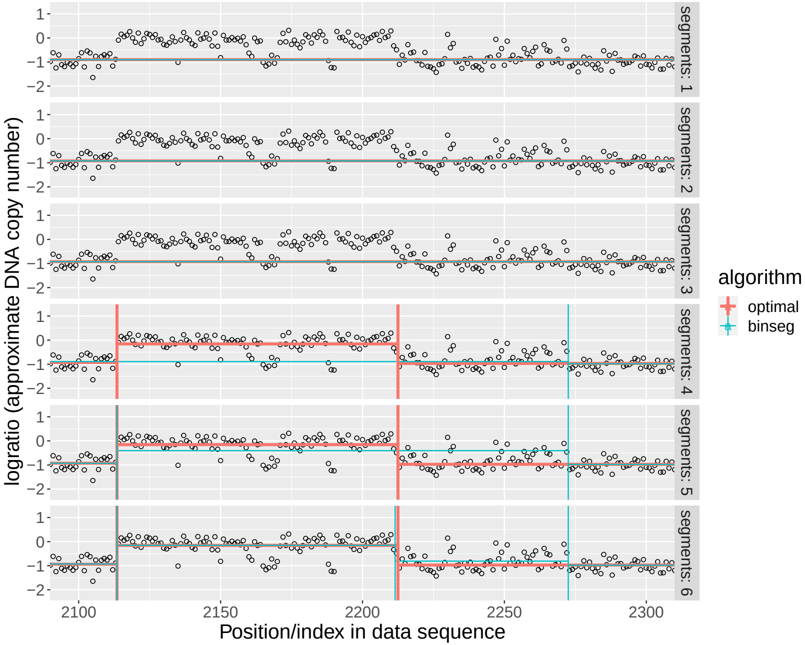
Example 1: stuck with sub-optimal change



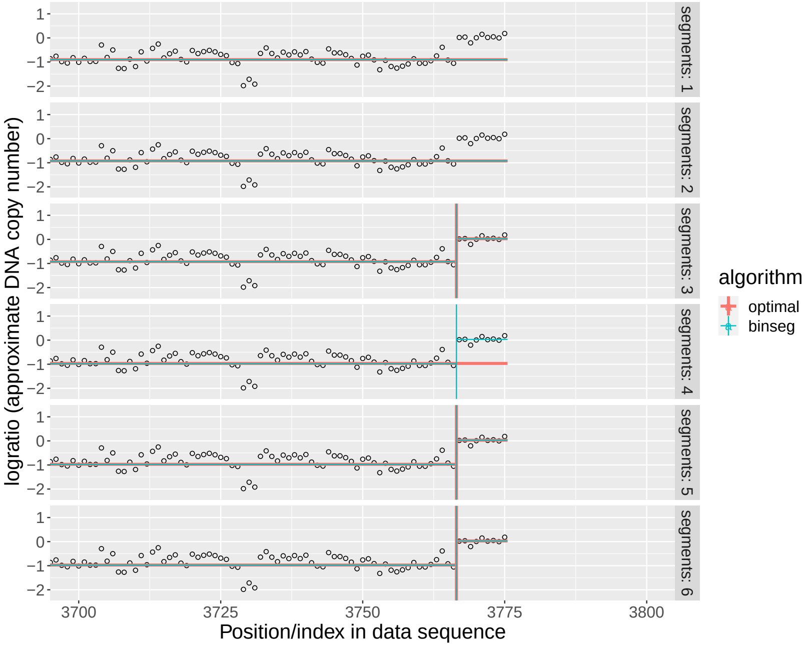
Zoom to start



Zoom to center

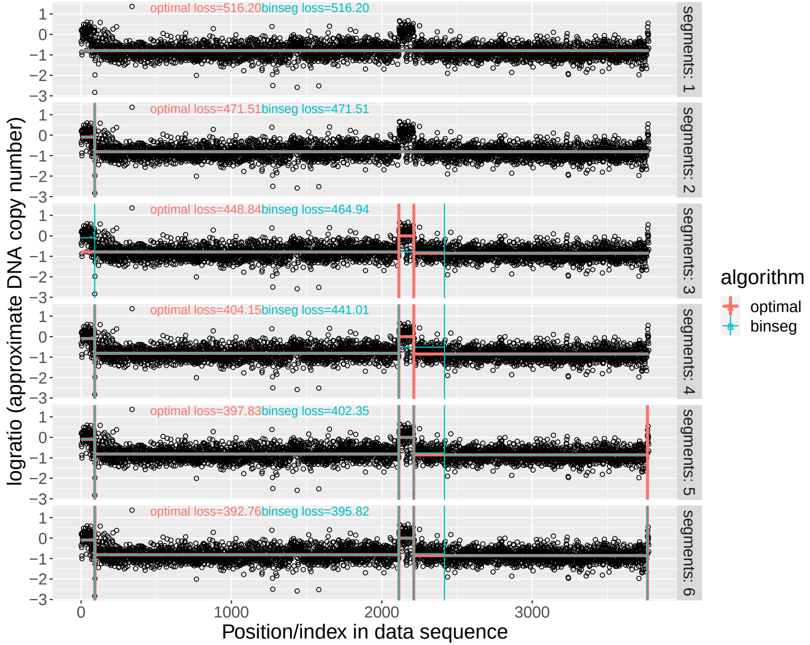


Zoom to end

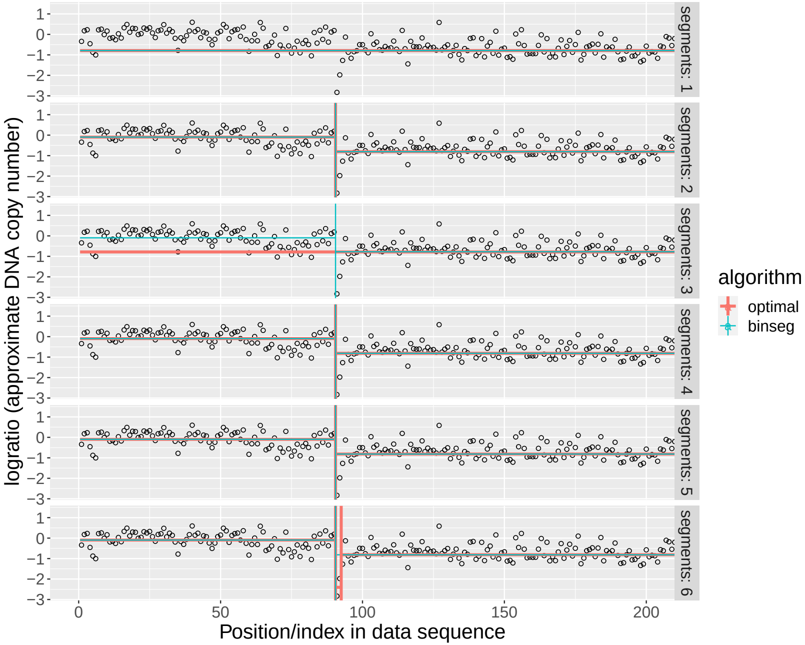


logratio (approximate DNA copy number)
Position/index in data sequence
3700
3725
3750
3775
3800
1
0
−1
−2
segments: 1
segments: 2
segments: 3
segments: 4
segments: 5
segments: 6
algorithm
optimal
binseg

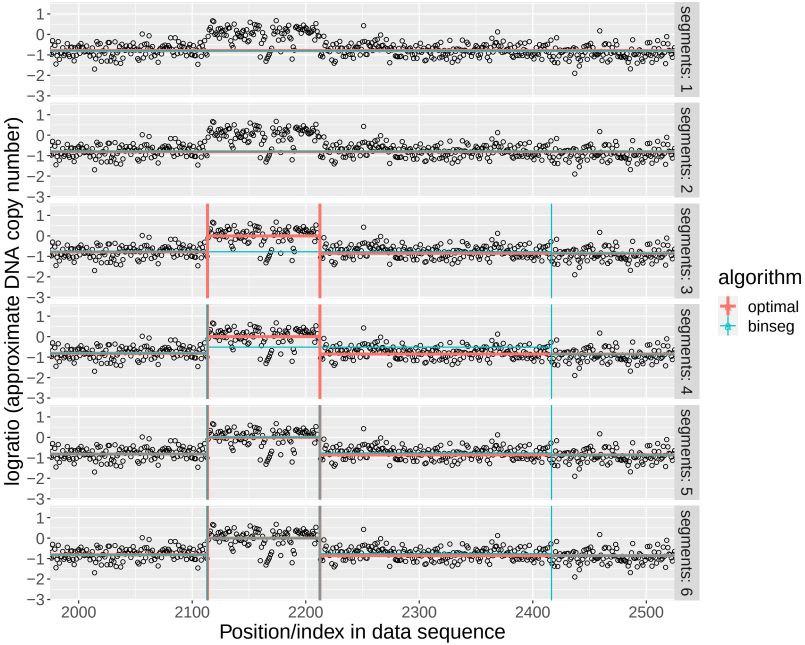
Example 2: missing a small change down



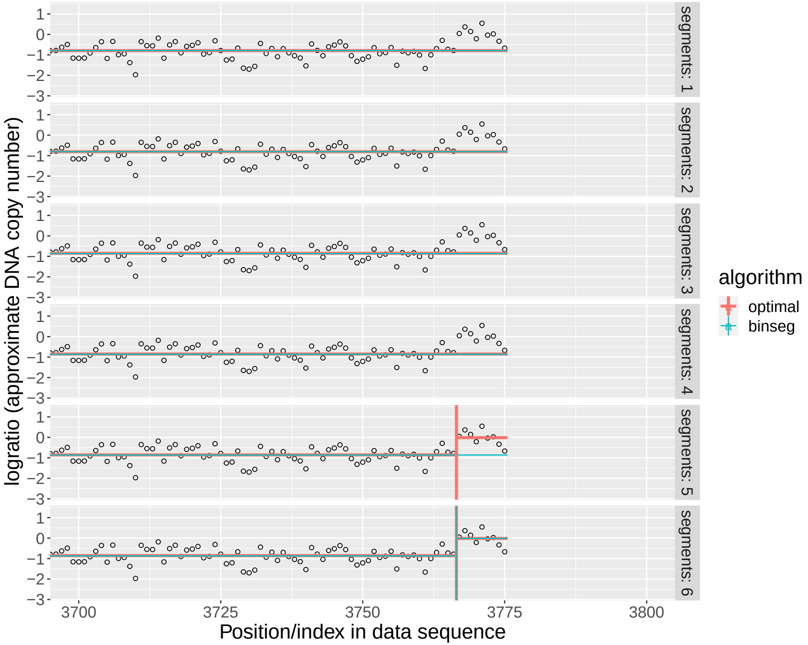
Zoom to start



Zoom to center



Zoom to end



1
0
−1
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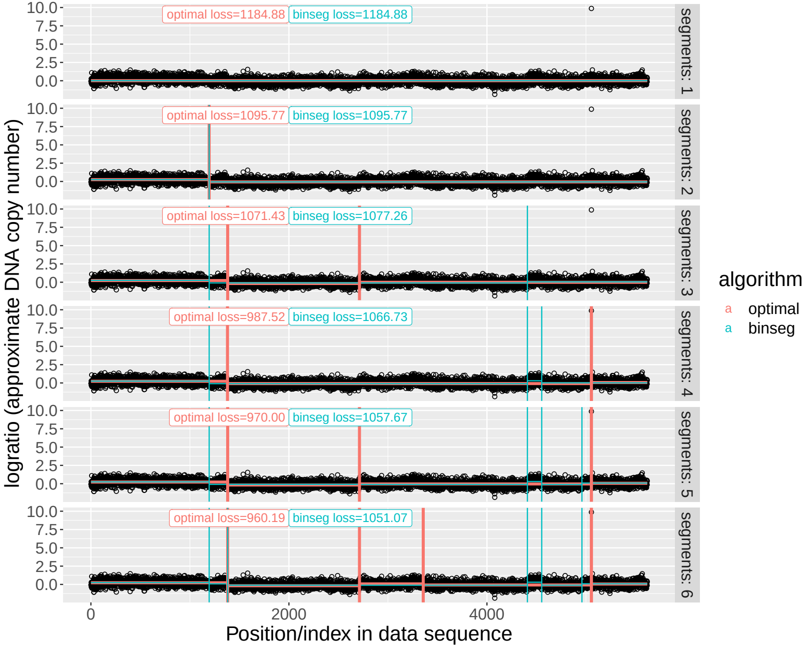
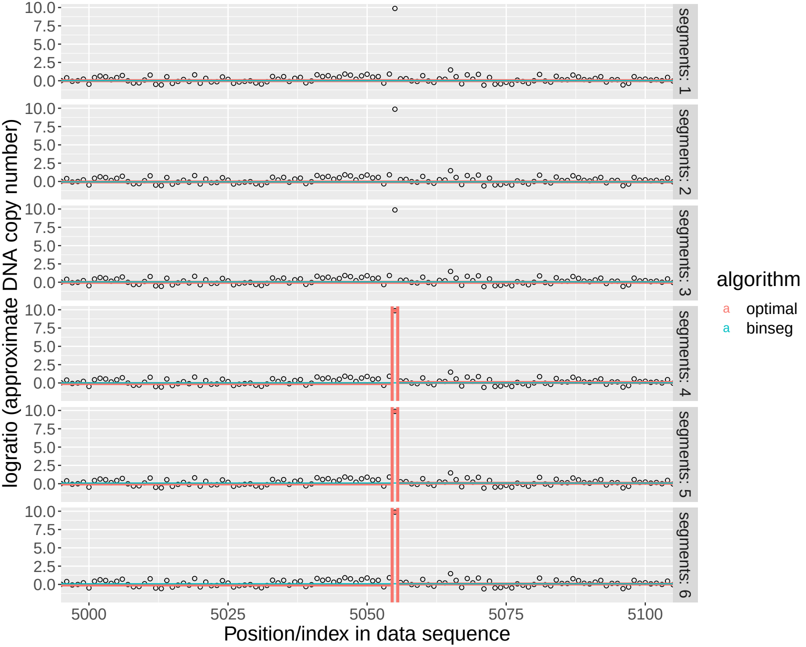
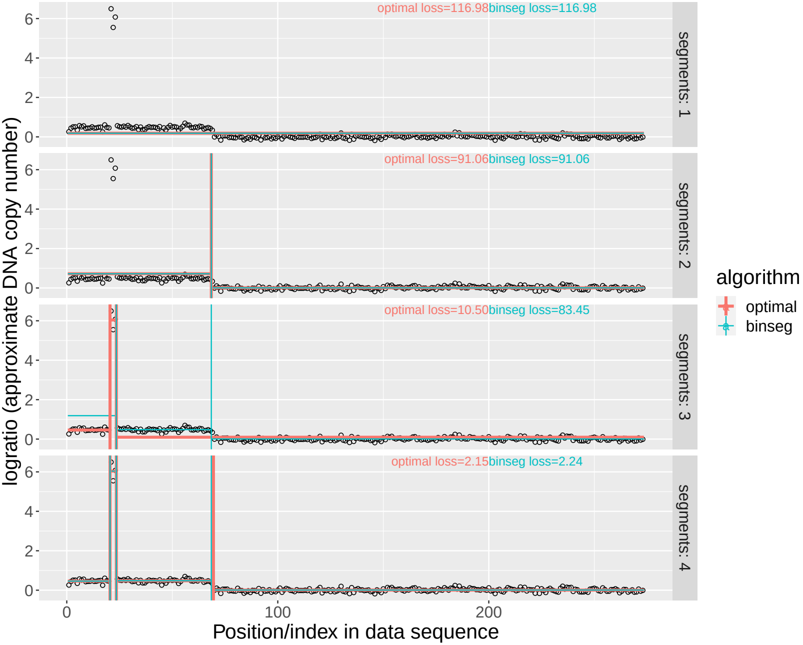
Example 3: difficult to detect an outlier



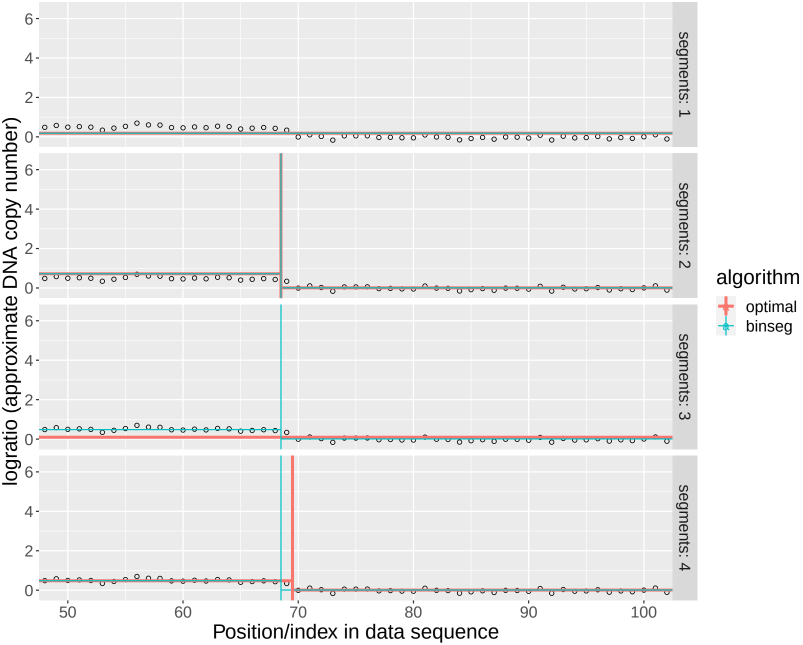
Zoom X axis to outlier



Example 4: stuck with sub-optimal change

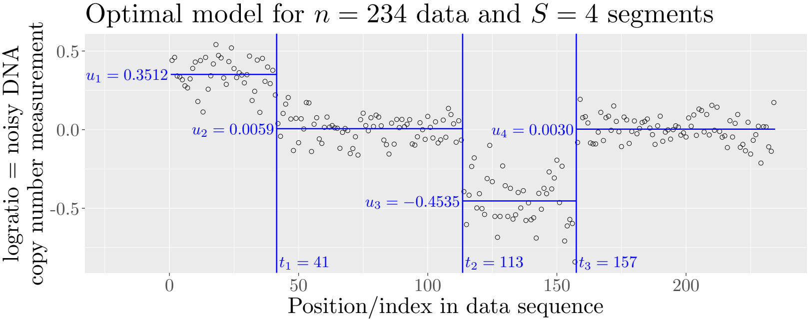


Zoom to changepoint



Dynamic programming for optimal changepoint detection

- We have n data $z_1, \dots, z_n$.
- Fix the number of segments $S \in \{1, 2, \dots, n\}$.
- Optimization variables: $S - 1$ changepoints $t_1 < \cdots < t_{S-1}$ and S segment means $u_1, \dots, u_S \in \mathbb{R}$ ($t_0 = 0$, $t_S = n$).
- Statistical model: for every segment $s \in \{1, \dots, S\}$, $z_i \overset{\text{iid}}{\sim} N(u_s, \sigma^2)$ for every data point $i \in (t_{s-1}, t_s]$ implies square loss function $\ell(u_s, z_i) = (u_s - z_i)^2$ to minimize.



Maximum likelihood inference for S segments and n data

The best loss for S segments and n data is

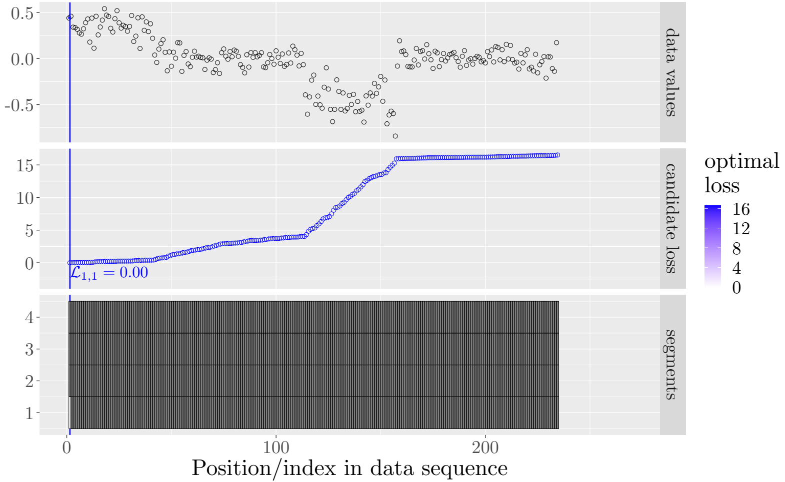
$$\begin{aligned}
\mathcal{L}_{S,n} &= \min_{\substack{\mathbf{u}\in\mathbb{R}^S \\ 0=t_0<t_1<\cdots<t_{S-1}<t_S=n}} \sum_{s=1}^{S} \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i) \\
&= \min_{t_{S-1}} \underbrace{\min_{\substack{u_1,\dots,u_{S-1} \\ t_1<\cdots<t_{S-2}}} \sum_{s=1}^{S-1} \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i)}_{\mathcal{L}_{S-1,t_{S-1}}} + \underbrace{\min_{u_S} \sum_{i=t_{S-1}+1}^{t_S=n} \ell(u_S, z_i)}_{c_{(t_{S-1},t_S=n]}}
\end{aligned}$$

- Hard optimization problem because of integer-valued changepoint t_s variables, naively $O(n^S)$ time.
- Auger and Lawrence (1989): $O(Sn^2)$ time classical dynamic programming algorithm (best loss computed recursively).

$$\mathcal{L}_{s,t} = \min_{t'<t} \mathcal{L}_{s-1,t'} + c_{(t',t]}$$

Initialization of dynamic programming

$$\mathcal{L}_{1,t} = c_{(0,t]}$$



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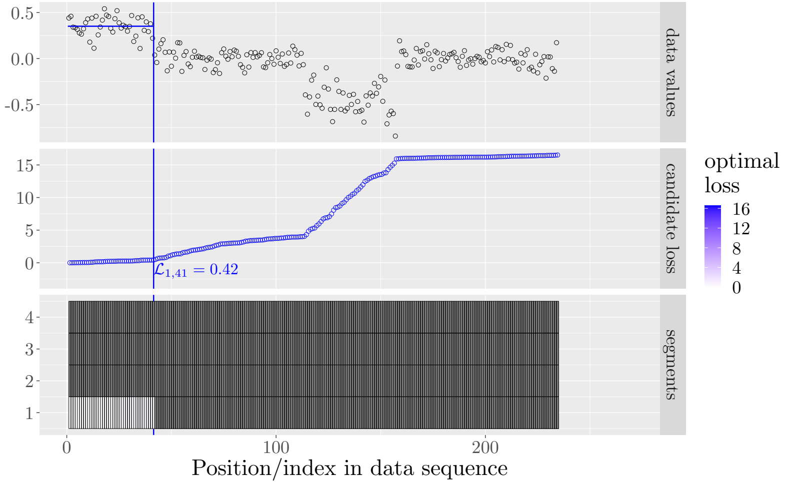

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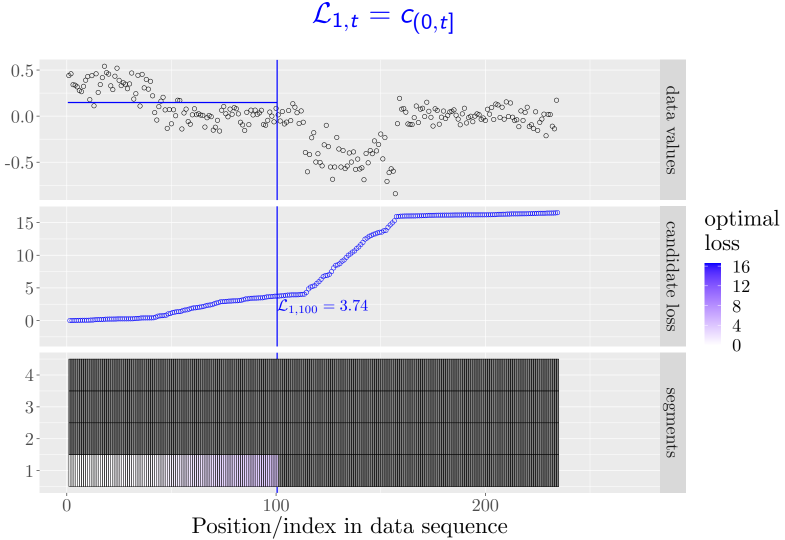

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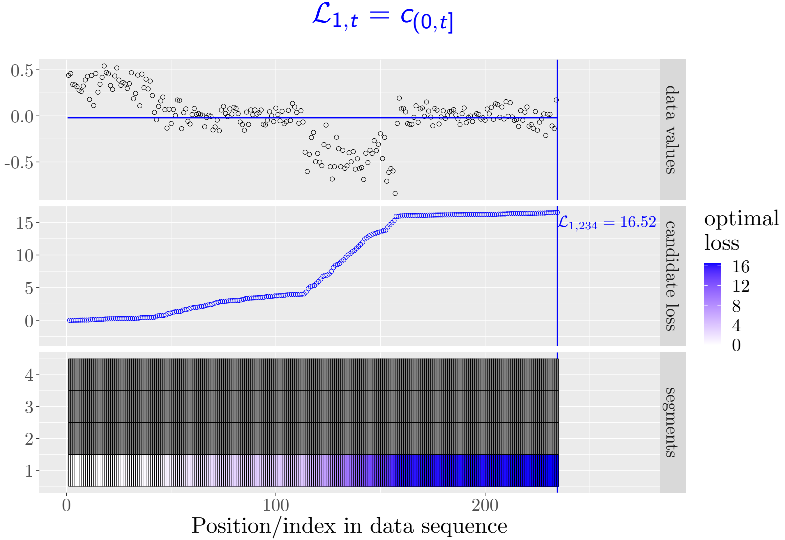


Efficient computation of c values

The best square loss up to t is

$$c_{(0,t]} = \min_u \sum_{i=1}^{t} (z_i - u)^2 = \sum_{i=1}^{t} z_i^2 - \min_u 2\hat{u} \sum_{i=1}^{t} z_i + t\hat{u}^2.$$

We can use cumulative sum to compute S_t for all t in linear $O(t)$ time, $S_t = \sum_{i=1}^{t} z_i$.

And best means up to t, $\hat{u}_t = S_t/t$.

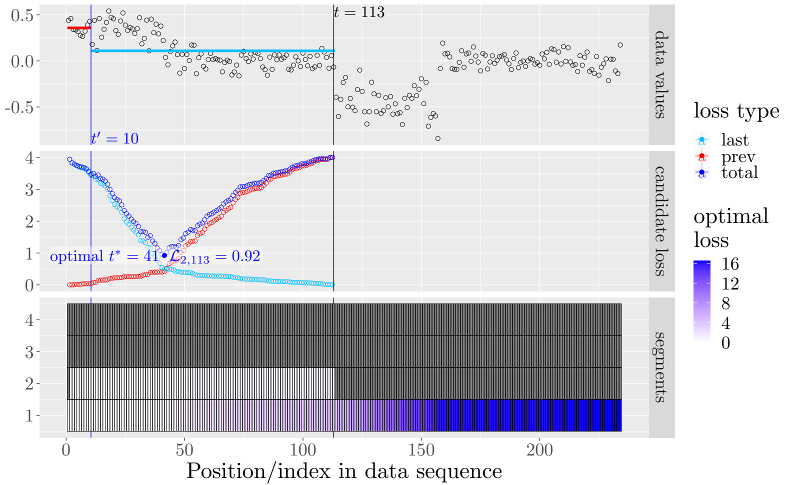
And cumulative sum of squares, $Q_t = \sum_{i=1}^{t} z_i^2$.

And best loss up to t,

$$\sum_{i=1}^{t} z_i^2 - 2\hat{u}_t \sum_{i=1}^{t} z_i + t\hat{u}_t^2 = Q_t - 2(S_t/t)(S_t) + t(S_t/t)^2 = Q_t - S_t^2/t.$$

First iteration/changepoint of dynamic programming

$$\mathcal{L}_{2,t} = \min_{t'<t} \mathcal{L}_{1,t'} + c_{(t',t]}$$



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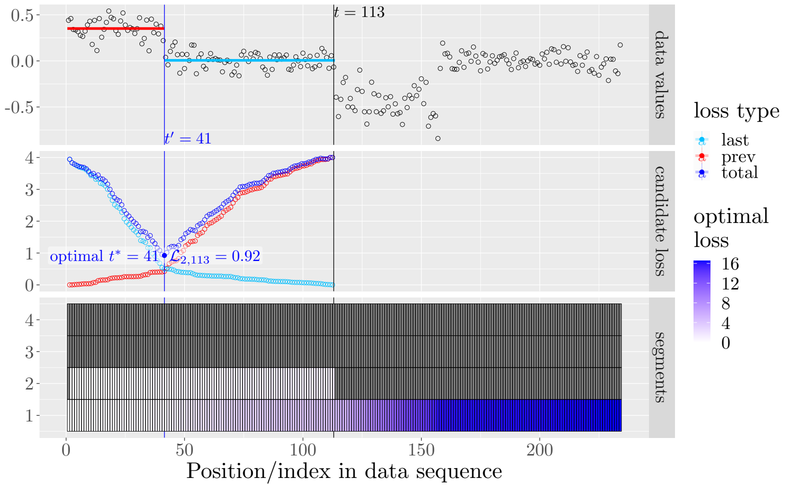

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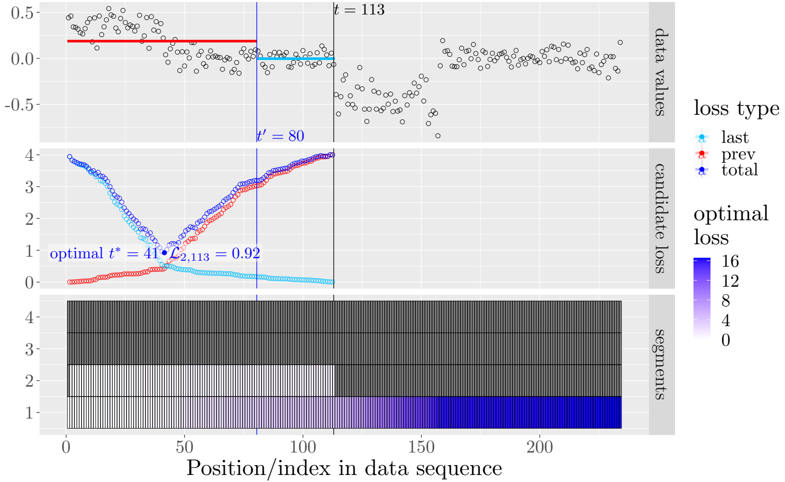

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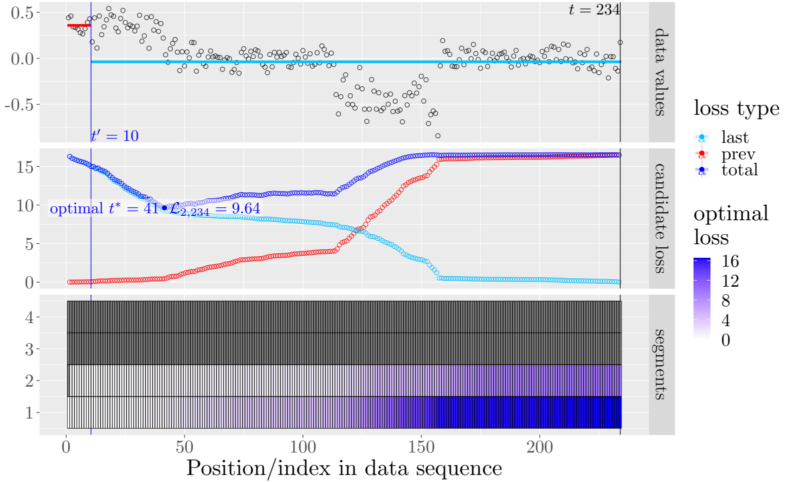

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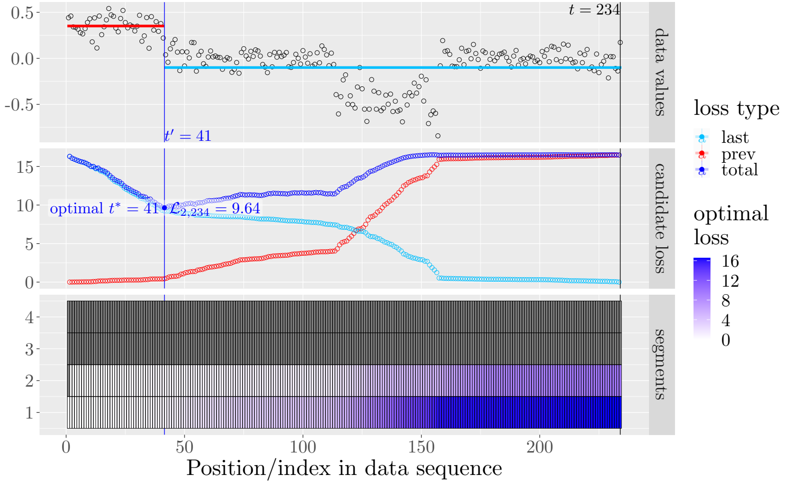

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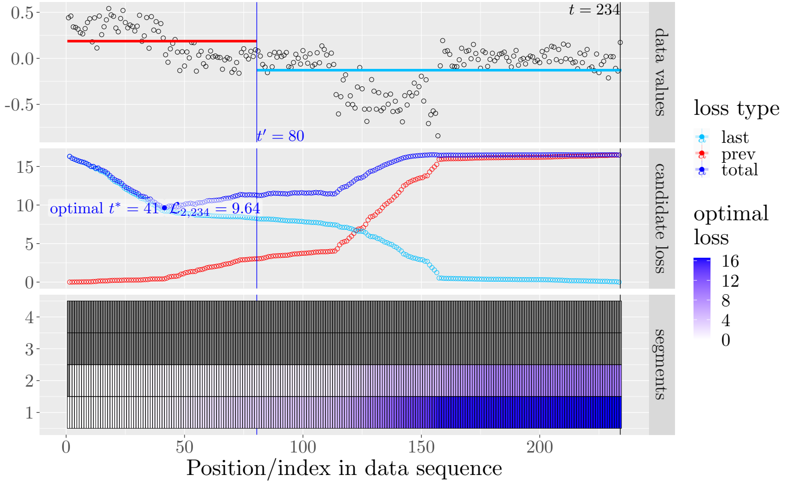

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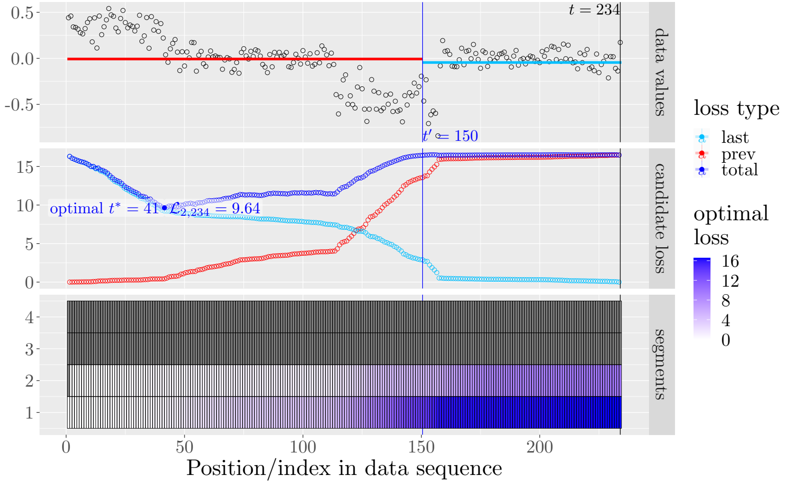


Time complexity for S segments and n data

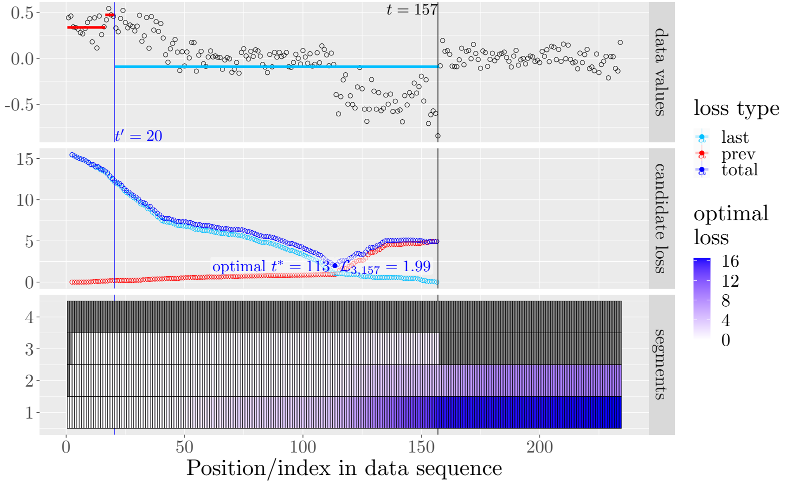
changes	naive	DP(classic)	DP(pruned)	BinSeg
1	$O(n)$	$O(n)$	$O(n)$–$O(n^2)$	$O(n)$
2	$O(n^2)$	$O(n^2)$	$O(n)$–$O(n^2)$	$O(\log n)$–$O(n)$
3	$O(n^3)$	$O(n^2)$	$O(n)$–$O(n^2)$	$O(\log n)$–$O(n)$
4	$O(n^4)$	$O(n^2)$	$O(n)$–$O(n^2)$	$O(\log n)$–$O(n)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	

Dynamic programming with either functional or inequality pruning leads to asymptotic speedups, see Maidstone R, Hocking TD, Rigaill G, Fearnhead P. On optimal multiple changepoint algorithms for large data. Statistics and Computing (2016).

Space: DP stores $O(nS)$ loss $\mathcal{L}_{s,t}$ values (always), BinSeg stores $O(S)$ split candidates (worst case).

Second iteration/changepoint of dynamic programming

$$\mathcal{L}_{3,t} = \min_{t'<t} \mathcal{L}_{2,t'} + c_{(t',t]}$$



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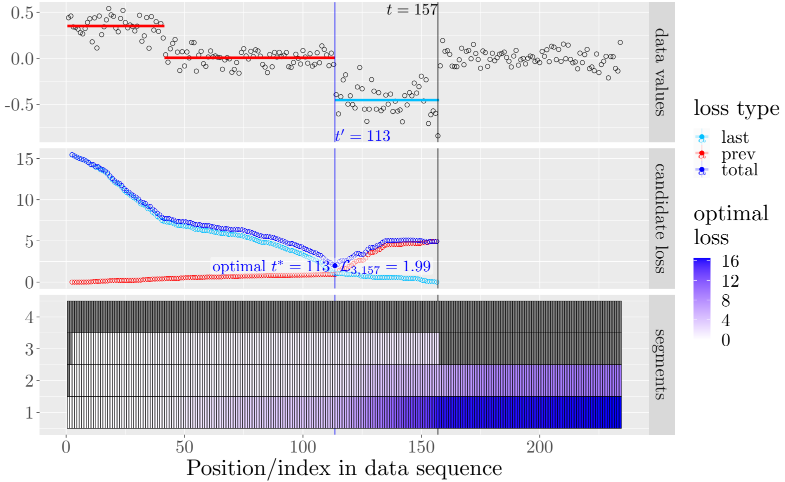

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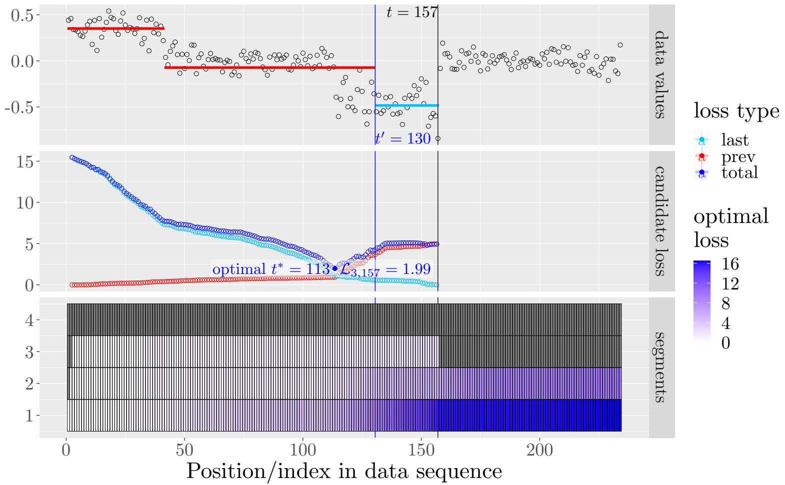
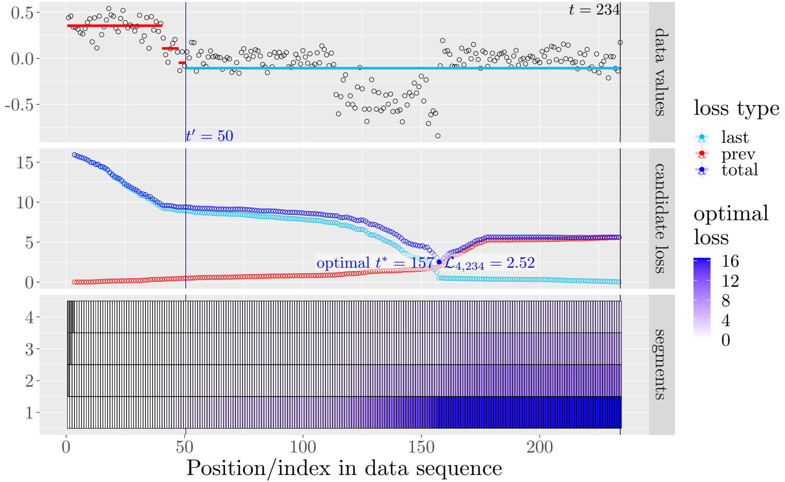


Third iteration/changepoint of dynamic programming

$$\mathcal{L}_{4,t} = \min_{t'<t} \mathcal{L}_{3,t'} + c_{(t',t]}$$



Third iteration/changepoint of dynamic programming

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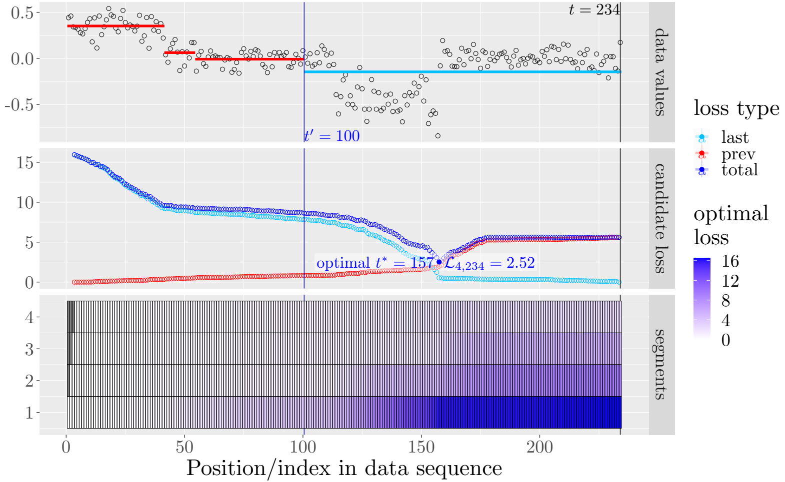

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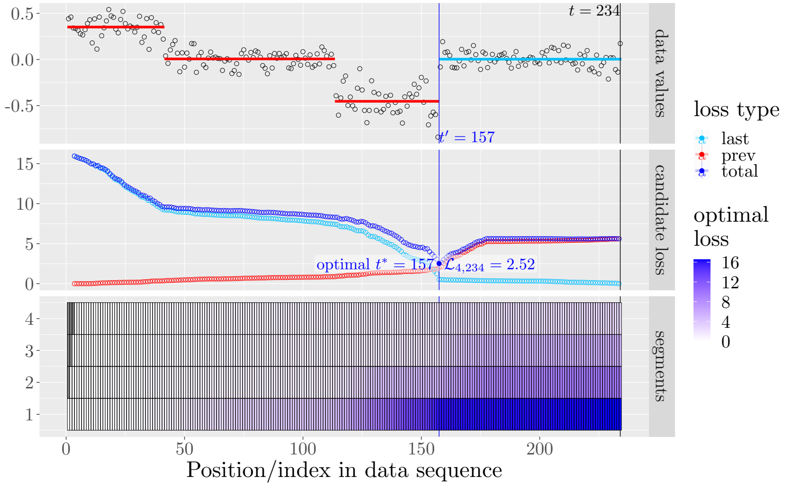

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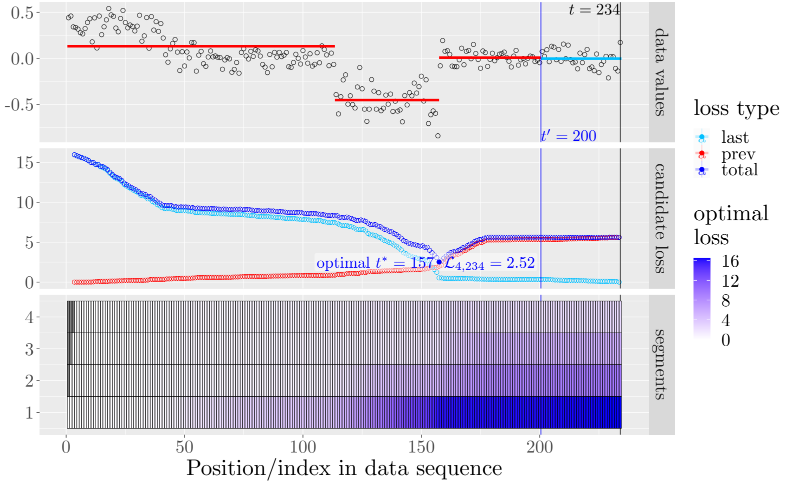

Comparison with previous approximate/heuristic algorithms

Every other algorithm we have seen so far has been approximate/heuristic, because it is not guaranteed to compute a global optimum of the objective function.

- K-means: local minimum squared error.
- EM algo for Gaussian mixtures: local maximum likelihood.
- Binary segmentation: local minimum squared error (maximum Gaussian likelihood).

In contrast the dynamic programming algorithm is guaranteed to compute a solution (segment means and changepoints) which is globally optimal (maximum Gaussian likelihoood, minimum squared error).

Dynamic programming is $O(n^2 S)$ for S segments and n data, whereas binary segmentation is $O(n \log S)$ best case and $O(nS)$ worst case. (optimal algorithms are typically slower than approximate/heuristic algorithms)

Other optimal algorithms

So far we have only discussed the *constrained problem*: hyper-parameter is number of segments $S \in \{1, \dots, n\}$.

An alternative formulation involves specifying a non-negative penalty hyper-parameter, $\lambda \in \mathbb{R}^+$, and then solving the *penalized problem*:

$$\min_{m_1,\dots,m_n \in \mathbb{R}} \underbrace{\sum_{i=1}^{n} \ell(m_i, z_i)}_{\text{loss}} + \lambda \underbrace{\sum_{i=1}^{n-1} I[m_i \neq m_{i+1}]}_{\text{number of changes}}.$$

The resulting model is the solution to a constrained problem (for some number of segments S).

Dynamic programming can also be used to solve this problem, using $O(n)$ space, best case $O(n)$ time (PELT algorithm), worst case $O(n^2)$ time. Optimal Detection of Changepoints With a Linear Computational Cost Killick R, Fearnhead P and Eckley IA. Journal of the American Statistical Association (2012).

Possible exam questions

- For S segments how does the binary segmentation loss compare to the dynamic programming loss? Answer for each $S \in \{1, 2, 3, 4\}$ one or more of: less than, equal, and/or greater than.
- How many values for the last changepoint variable are considered in the computation of $\mathcal{L}_{3,100}$?
- Is $\{$binary segmentation, dynamic programming$\}$ an $\{$optimal, approximate$\}$ algorithm? Why?