Binary segmentation

Toby Dylan Hocking

Motivation for changepoint detection in time series data

- Detecting changes/abnormalities important in medicine.

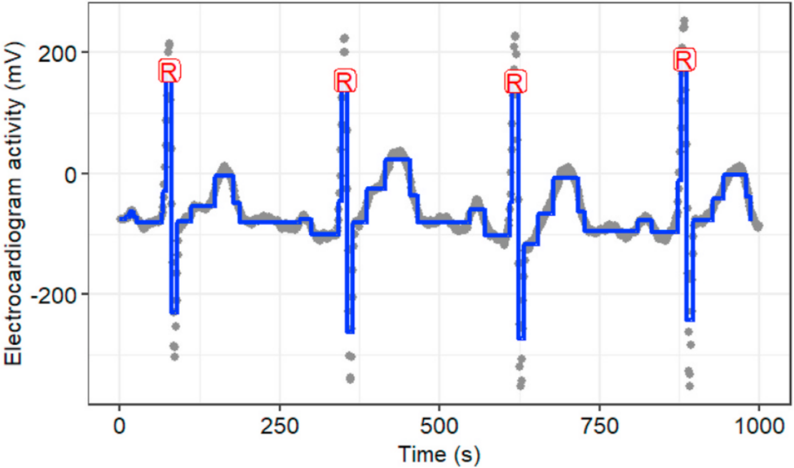


Figure 1: Electrocardiograms (heart monitoring), Fotoohinasab et al, Asilomar conference 2020.

Motivation for changepoint detection in time series data

- Detecting the time when a spike occurs is important in neuroscience.

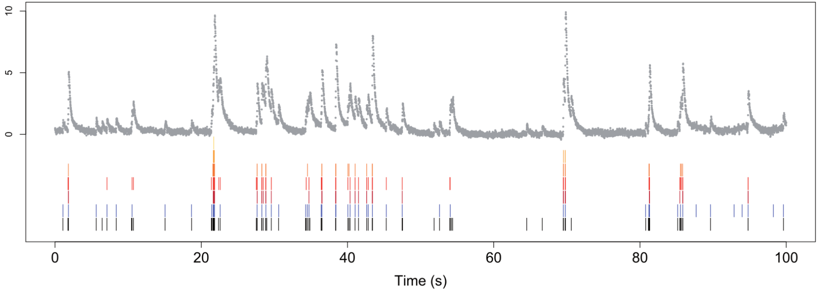


Figure 2: Neural spikes in calcium imaging data, Jewell et al, Biostatistics 2019.

Motivation for changepoint detection in genomic data sequences

- Detecting breakpoints is important in diagnosis of some types of cancer, such as neuroblastoma.

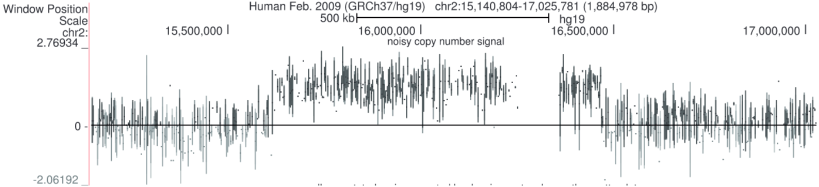


Figure 3: DNA copy number data, breakpoints associated with aggressive cancer, Hocking et al, Bioinformatics 2014.

Motivation for changepoint detection in genomic data sequences

- Detecting peaks (up/down changes) in genomic data is important in order to understand which genes are active or inactive.

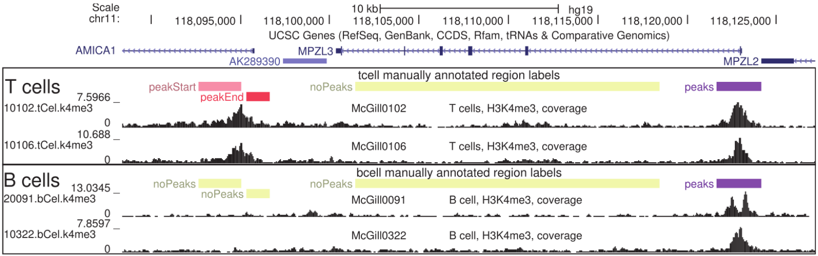


Figure 4: ChIP-seq data for characterizing active regions in the human genome, Hocking et al, Bioinformatics 2017.

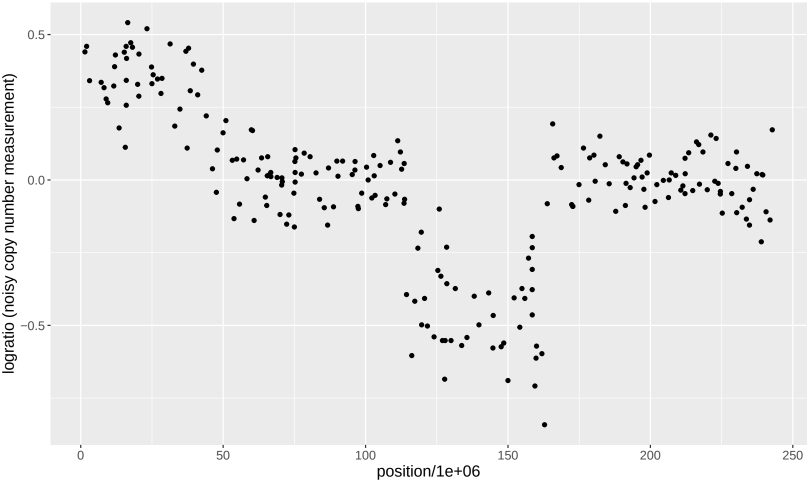
Segmentation / changepoint detection framework

- Let $x_1, \dots, x_n \in \mathbb{R}$ be a data sequence over space or time (logratio column in DNA copy number data below).
- Where are the abrupt changes in the data sequence?

```
##      profile.id chromosome  position    logratio
##          <fctr>     <fctr>     <int>       <num>
##   1:          4          2   1472476  0.44042072
##   2:          4          2   2063049  0.45943162
##   3:          4          2   3098882  0.34141652
##   4:          4          2   7177474  0.33571191
##   5:          4          2   8179390  0.31730407
##  ---
## 230:          4          2 239227603  0.01863417
## 231:          4          2 239471307  0.01720929
## 232:          4          2 240618997 -0.10935876
## 233:          4          2 242024751 -0.13764780
## 234:          4          2 242801018  0.17248752
```

Segmentation / changepoint data visualization

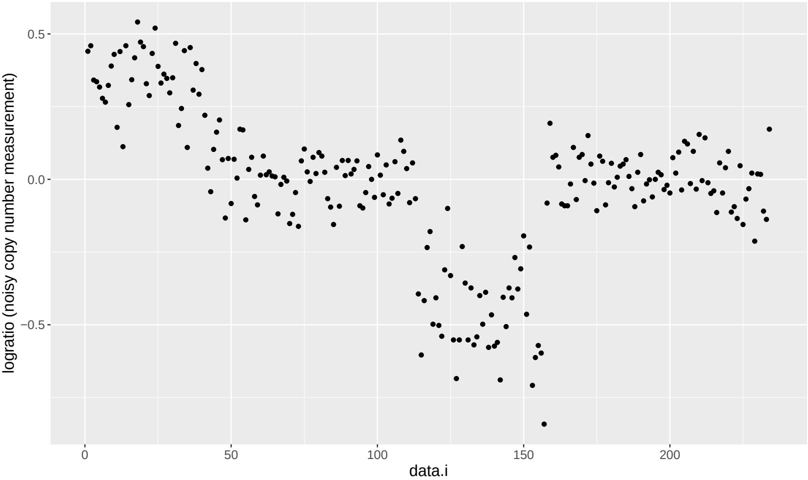
- Let $x_1, \dots, x_n \in \mathbb{R}$ be a data sequence over space or time.
- Where are the abrupt changes in the data sequence?



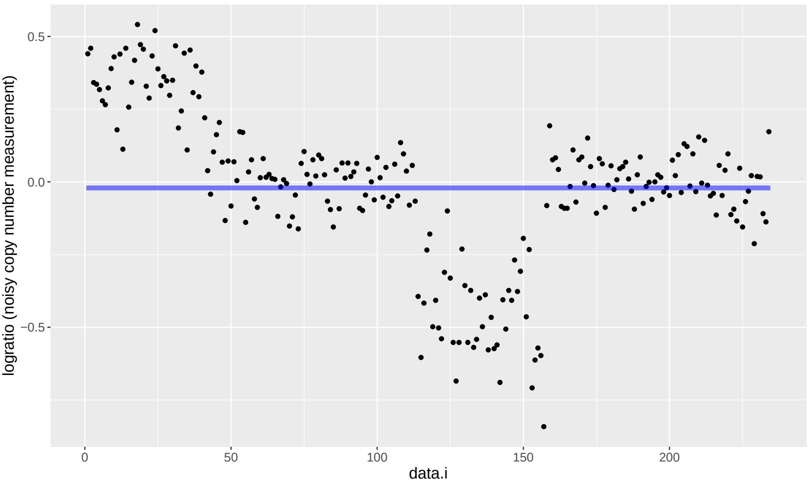
Assume normal distribution with change in mean, constant variance

- There are a certain number of clusters/segments $K \in \{1, \dots, n\}$.
- Each segment $k \in \{1, \dots, K\}$ has its own mean parameter $\mu_k \in \mathbb{R}$.
- There is some constant variance parameter $\sigma^2 > 0$ which is common to all segments.
- For each data point i on segment $k \in \{1, \dots, K\}$ we have $x_i \sim N(\mu_k, \sigma^2)$ – normal distribution.
- This normal distribution assumption means that we want to find segments/changepoints with mean m that minimize the square loss, $(x - m)^2$.
- Other distributional assumptions / loss functions are possible.

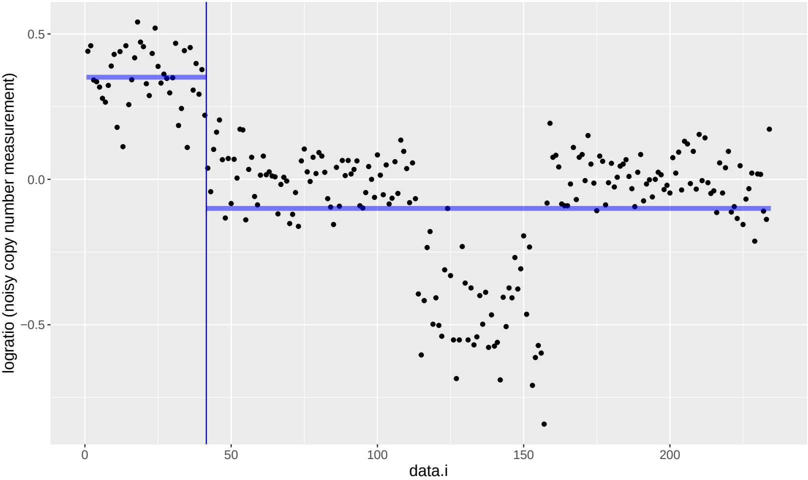
Visualize data sequence



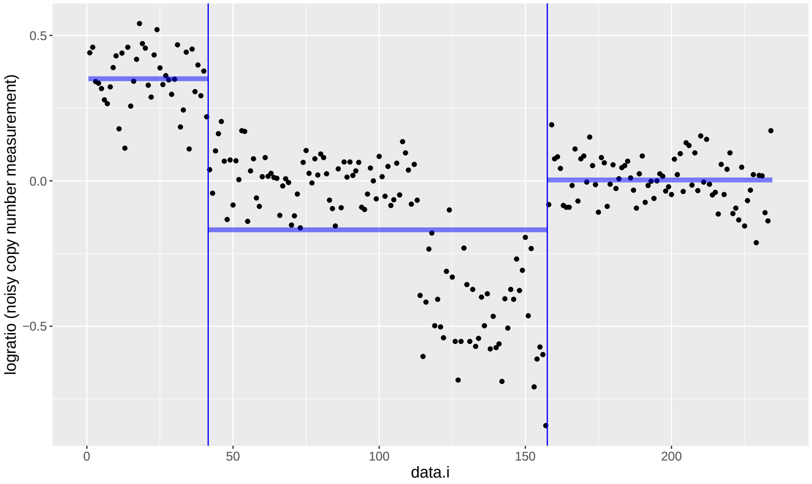
Simplest model, 1 segment, 0 changepoints



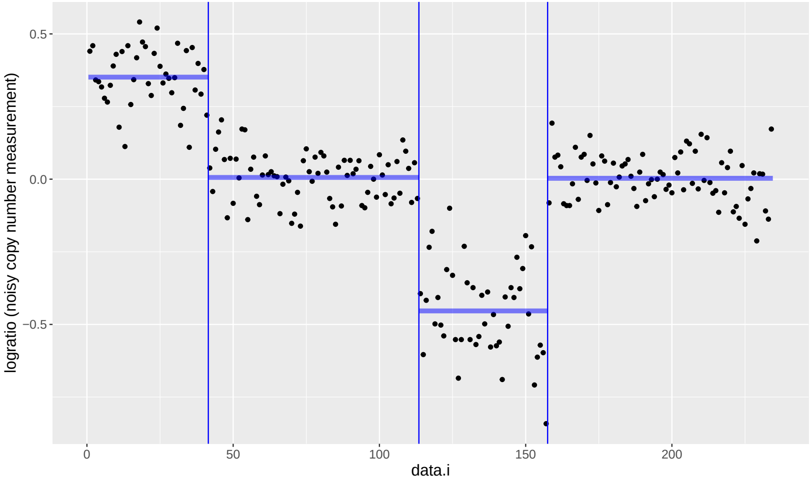
Find best single changepoint (two segments)



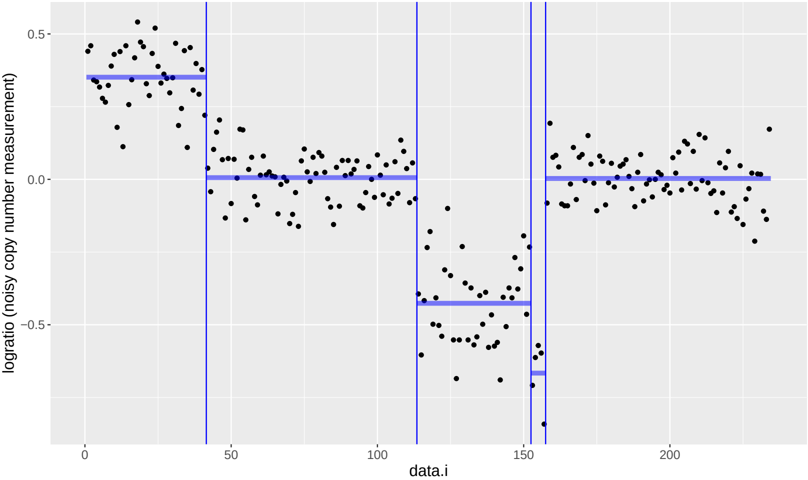
Find two changepoints (three segments)



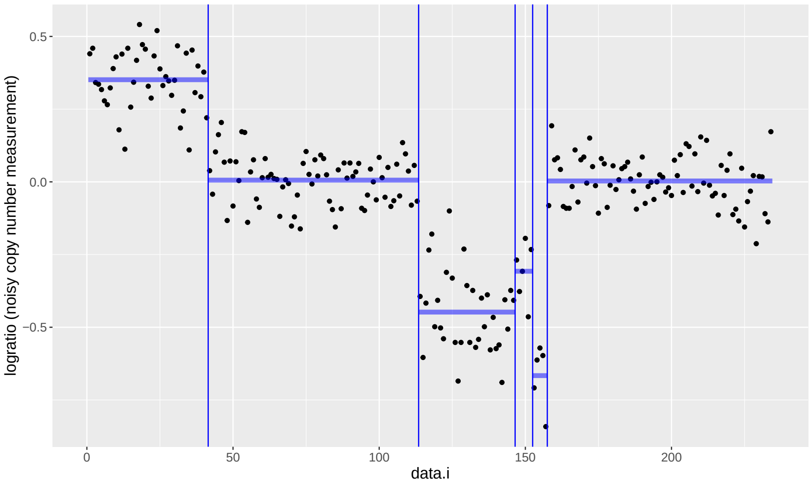
Find four segments



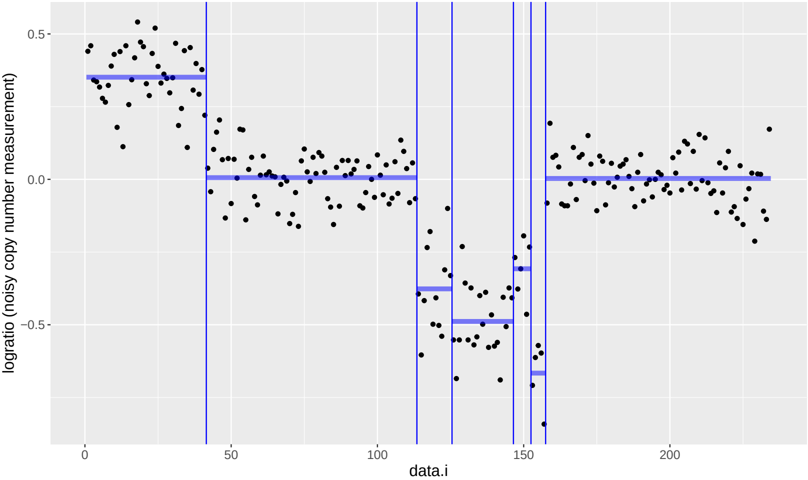
Find five segments



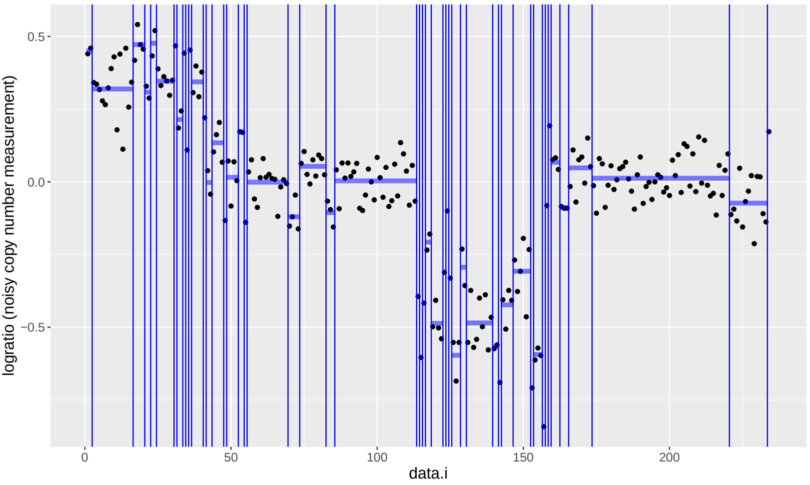
Find six segments



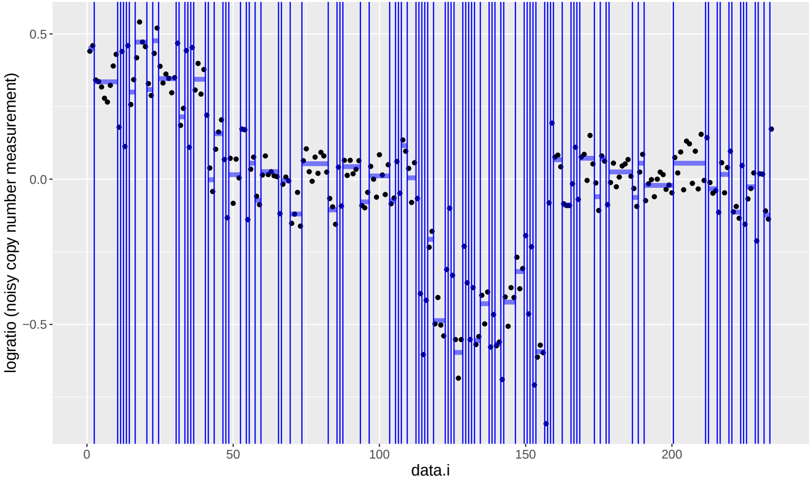
Find seven segments



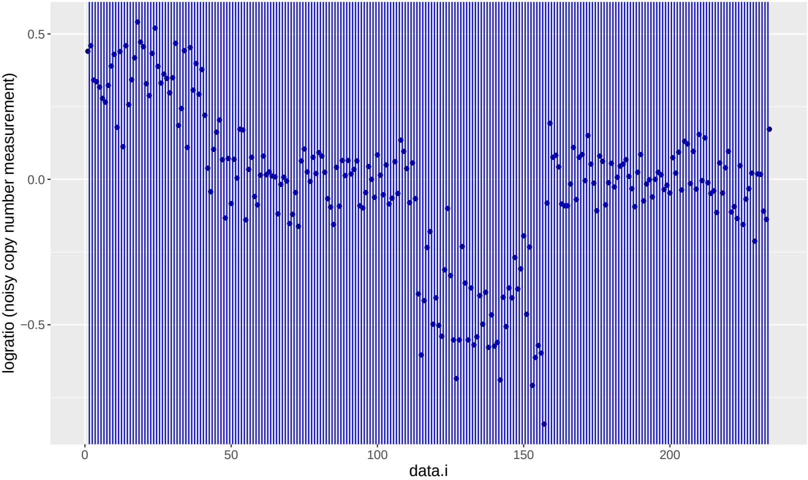
Find 50 segments



Find 100 segments

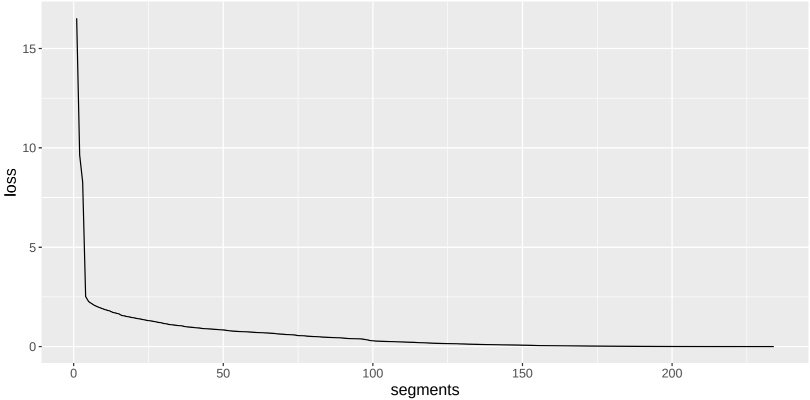


Largest model: 234 segments (changes everywhere)

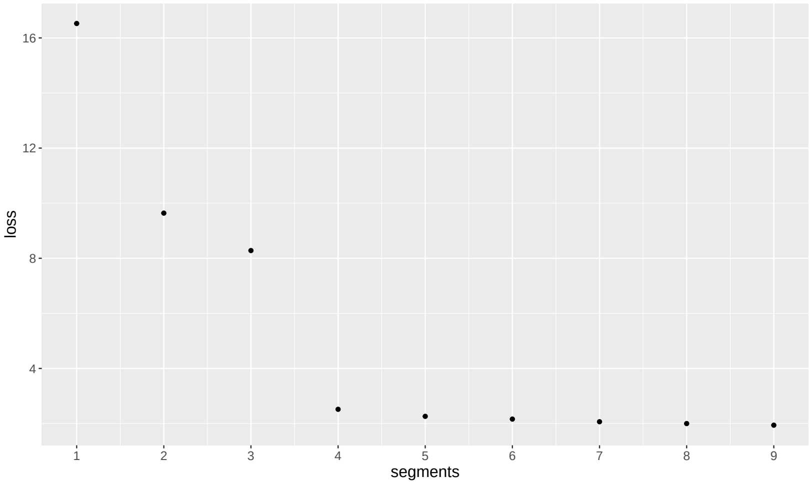


Error/loss function visualization

- Let $m^{(k)} \in \mathbb{R}^n$ be the mean vector with k segments.
- Error for k segments is defined as sum of squared difference between data x and mean $m^{(k)}$ vectors, $E_k = \sum_{i=1}^{n} (x_i - m_i^{(k)})^2$
- As in previous clustering models, kink in the error curve can be used as a simple model selection criterion.



Error/loss function zoom



Learning algorithm

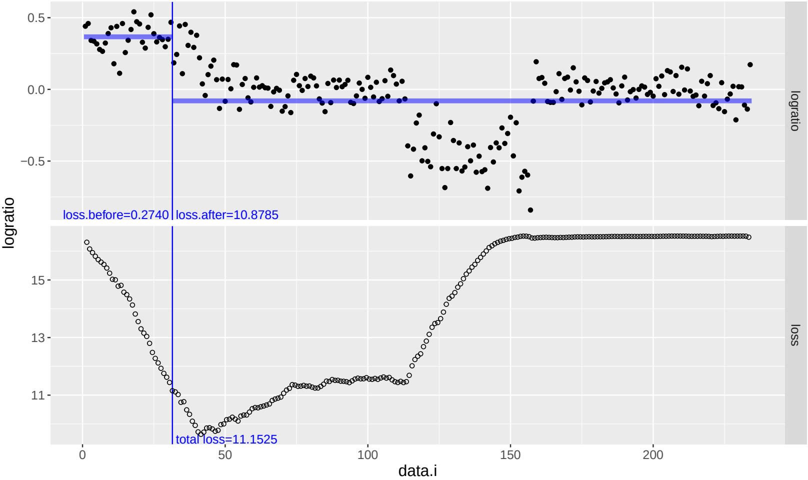
- Start with one segment, then repeat:
- Compute loss of each possible split.
- Choose split which results in largest loss decrease.
- If $s = \sum_{i=1}^{n} x_i$ is the sum over n data points, then the mean is s/n and the square loss (from 1 to n) is

$$L_{1,n} = \sum_{i=1}^{n} (x_i - s/n)^2 = \sum_{i=1}^{n} [x_i^2] - 2(s/n)s + n(s/n)^2$$

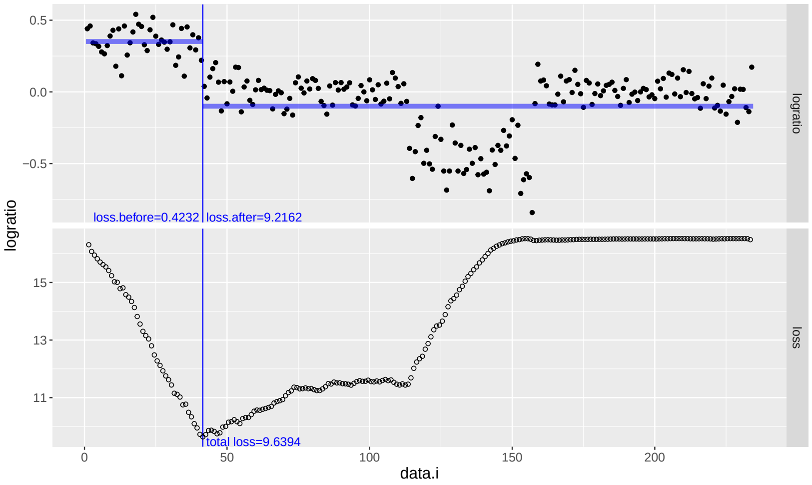
- Given cumulative sums, and a split point t, we can compute square loss from 1 to t, $L_{1,t}$, and from $t+1$ to n, $L_{t+1,n}$, in constant $O(1)$ time.
- We can minimize over all changepoints t in linear $O(n)$ time,

$$\min_{t \in \{1,\dots,n-1\}} L_{1,t} + L_{t+1,n}$$

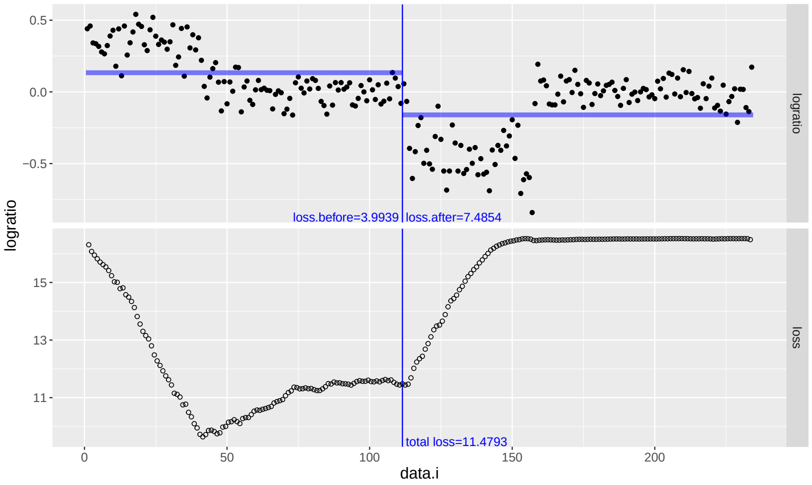
First step of binary segmentation



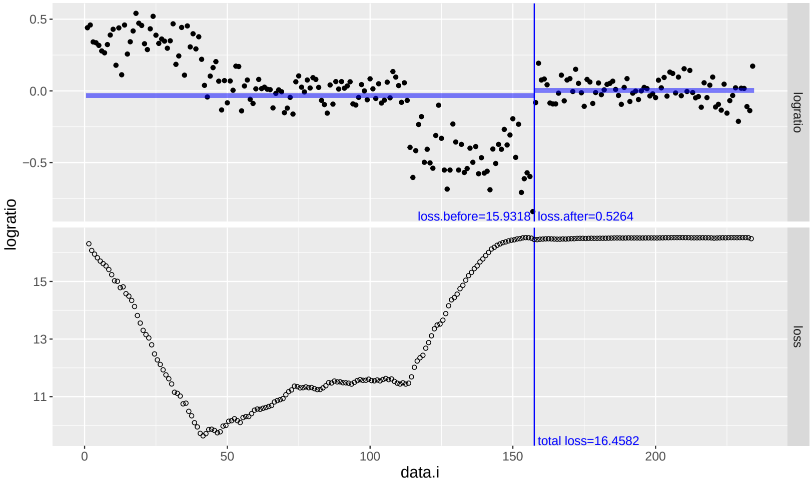
First step of binary segmentation



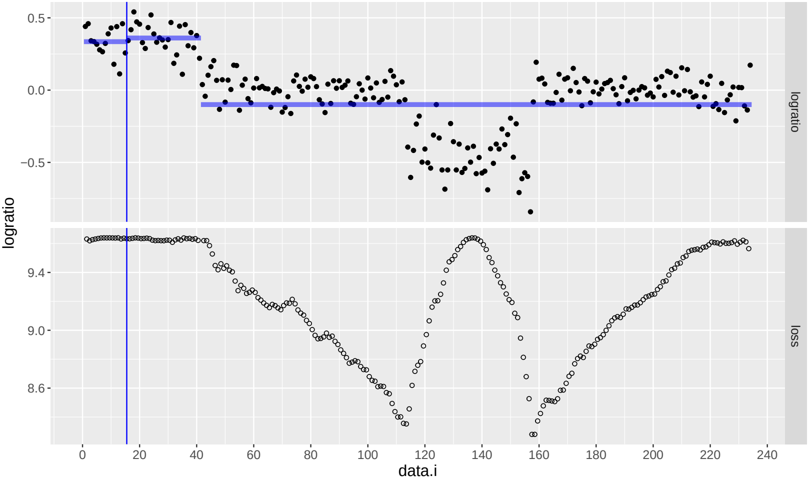
First step of binary segmentation



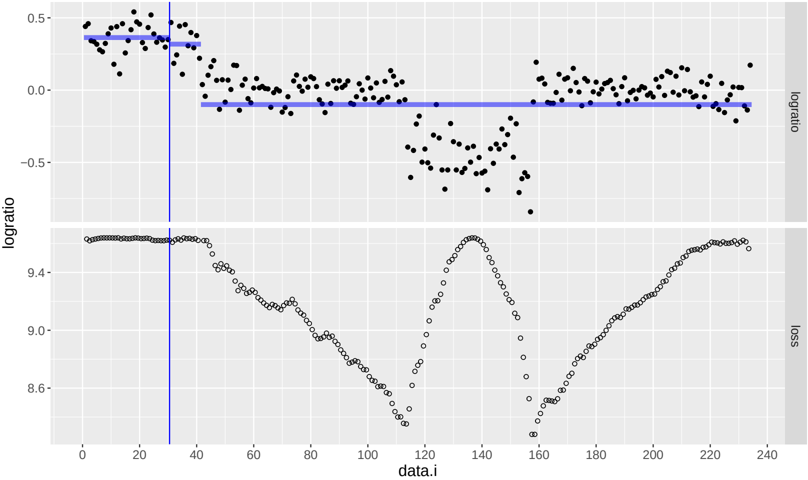
First step of binary segmentation



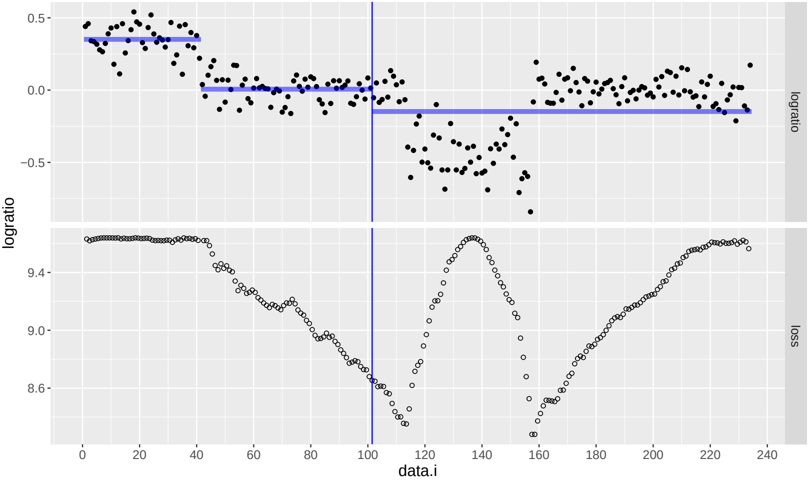
Second step of binary segmentation



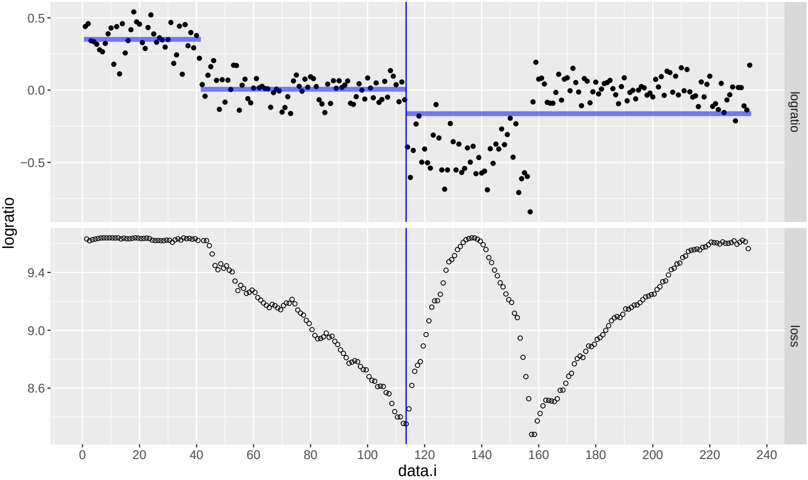
Second step of binary segmentation



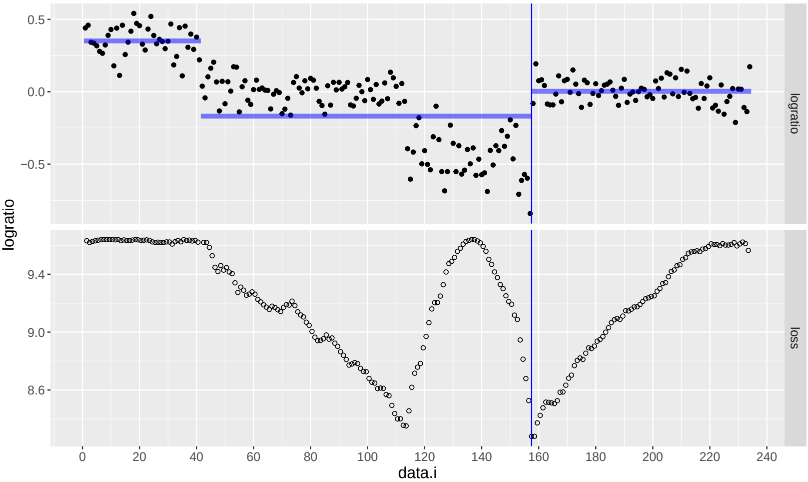
Second step of binary segmentation



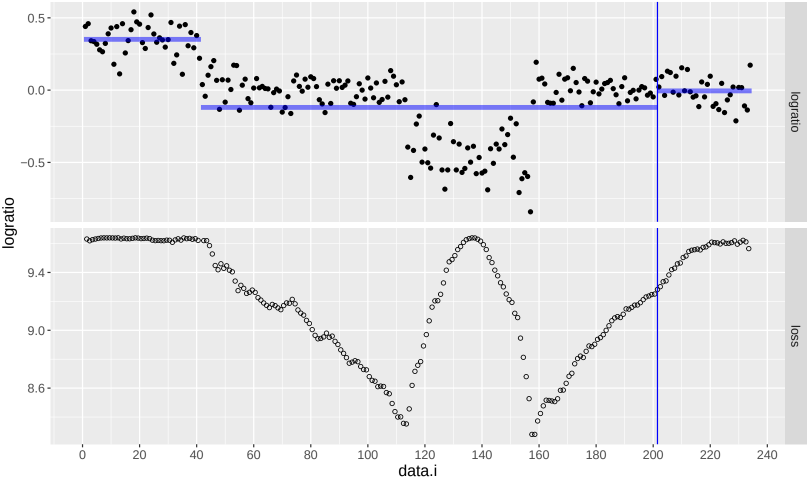
Second step of binary segmentation



Second step of binary segmentation

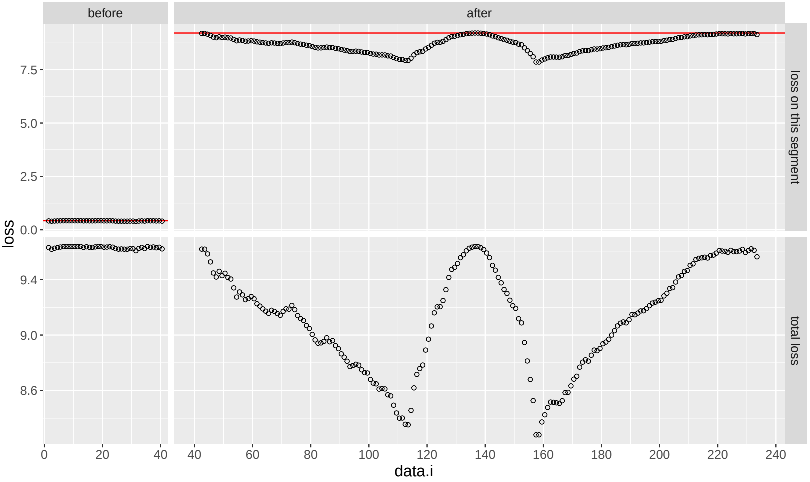


Second step of binary segmentation



Efficient loss computation

- Minimization can be performed by choosing the split with loss (black point) which maximizes the decrease in loss with respect to previous model (red, with no split).



Learning algorithm, implementation details

First compute the vectors of cumulative sums of data and squares, $y_1 = z_1 = 0, y_t = \sum_{i=1}^{t-1} x_i, z_t = \sum_{i=1}^{t-1} x_i^2$, for all $t \in \{2, \dots, n+1\}$.

Assume there is some set $\mathcal{S}$ of segments that could be split, each $(j, e) \in \mathcal{S}$ is a segment start j and end e (both in $1, \dots, n$).

Then the next segment to split (j, e), and best split point t, are defined by the best loss decrease,

$$\max_{(j,e)\in\mathcal{S}} \underbrace{L_{j,e}}_{\text{loss before split}} - \min_{t\in\{j,\dots,e-1\}} \underbrace{L_{j,t} + L_{t+1,e}}_{\text{loss after split}}$$

Use the cumsum trick to compute loss in constant time,

$$\sum_{i=j}^{t} x_i = y_{t+1} - y_j.$$

$$L_{j,t} = z_{t+1} - z_j - (y_{t+1} - y_j)^2/(t - j + 1).$$

Learning algorithm, recursion/pseudo-code

Notation. Let $D_{j,e}(t) = L_{j,t} + L_{t+1,n} - L_{j,e}$ be the loss difference after splitting segment (j, e) at t, and let $f(j, e) = \min, \arg\min_{t\in\{j,\dots,e-1\}} D_{j,e}(t)$ be the best loss difference/split on segment (j, e).

Initialization. Let $\mathcal{L}_1 = L_{1,n}$ be the loss with one segment, and let $\mathcal{S}_1 = \{(1, n, f(1, n))\}$ be the initial segment to split.

Recursion. For all $k \in \{2, \dots, K\}$: (max segments $K \leq n$)

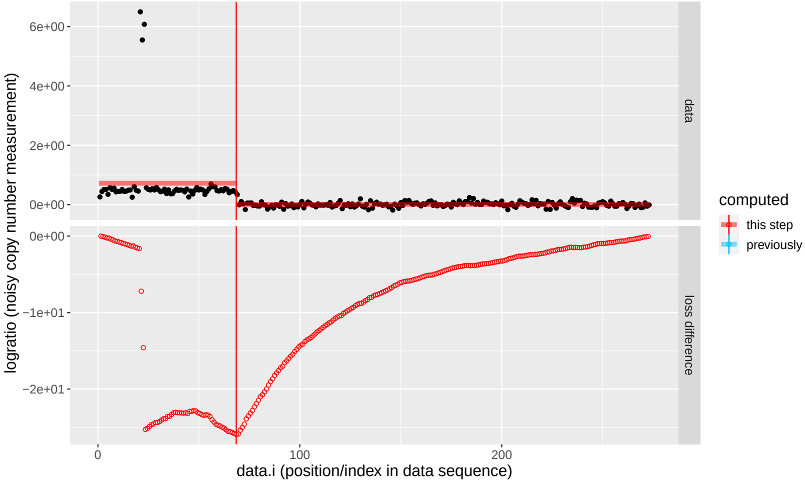
- $j_k^*, e_k^*, d_k^*, t_k^* = \arg\min_{(j,e,d,t)\in\mathcal{S}_{k-1}} d$ (best segment to split)
- $\mathcal{L}_k = \mathcal{L}_{k-1} + d_k^*$, (loss)
- $\mathcal{N}_k = \{(j_k^*, t_k^*), (t_k^* + 1, e_k^*)\}$ (new segments)
- $\mathcal{V}_k = \{(j, e, f(j, e)) \mid (j, e) \in \mathcal{N}_k, j < e\}$ (splittable segments)
- $\mathcal{S}_k = [\mathcal{S}_{k-1} \setminus (j_k^*, e_k^*, d_k^*, t_k^*)] \cup \mathcal{V}_k$ (segments to search)

Modification for min segment length

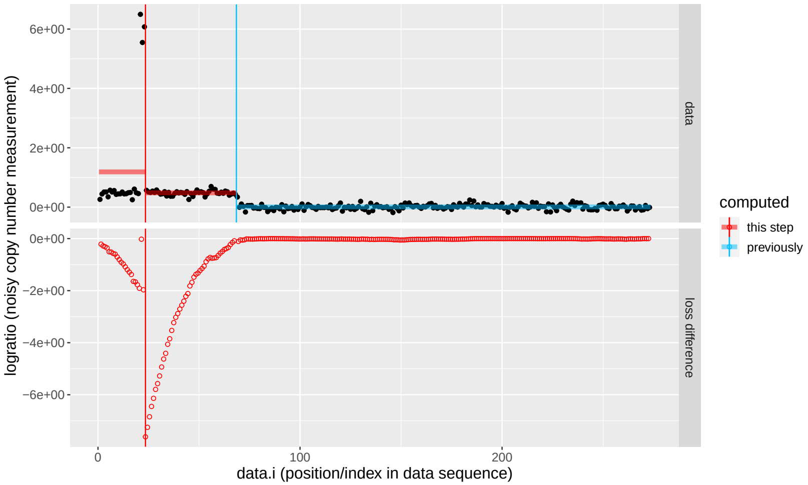
Sometimes there is prior knowledge that there should be no segments with fewer data points than $\ell \in \{1, 2, \dots\}$, and in that case there is a simple modification:

- $f(j,e) = \min, \arg\min_{t \in \{j+\ell-1,\dots,e-\ell\}} D_{j,e}(t)$ (best split)
- $\mathcal{V}_k = \{(j, e, f(j,e)) \mid (j,e) \in \mathcal{N}_k,\ e - j + 1 \geq 2\ell\}\}$ (splittable segments)

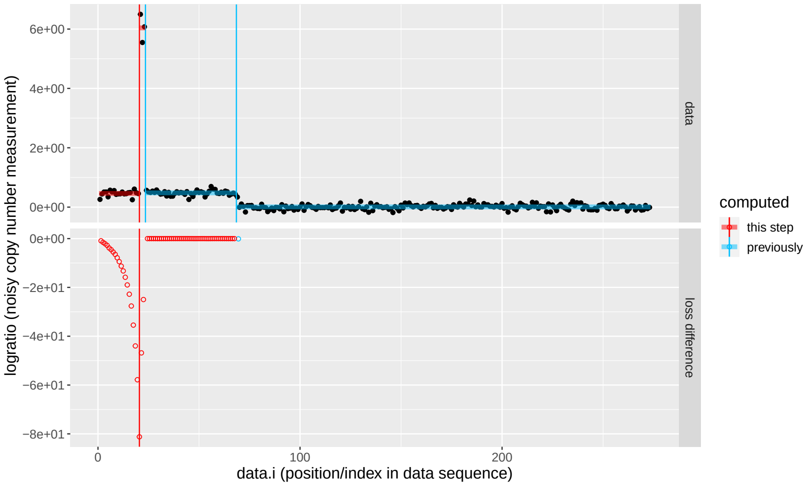
Visualization of computations at each iteration



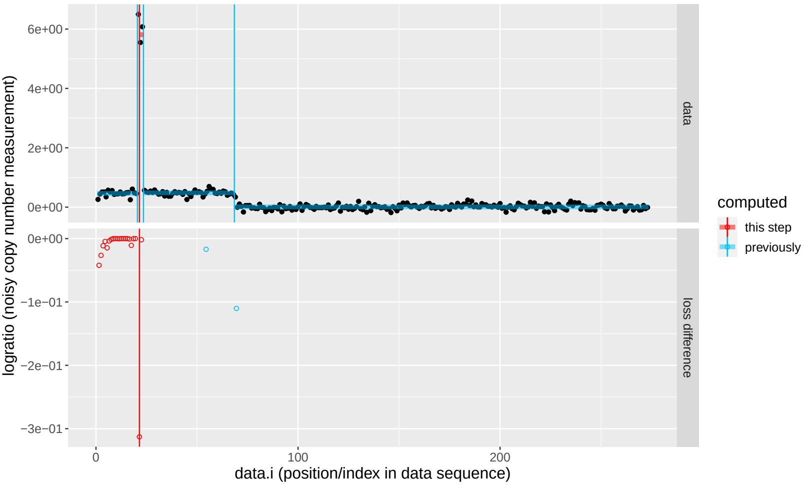
Visualization of computations at each iteration



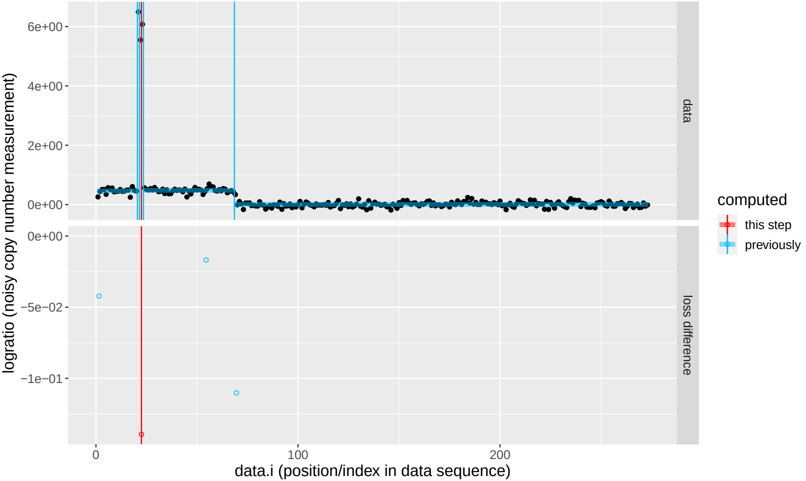
Visualization of computations at each iteration



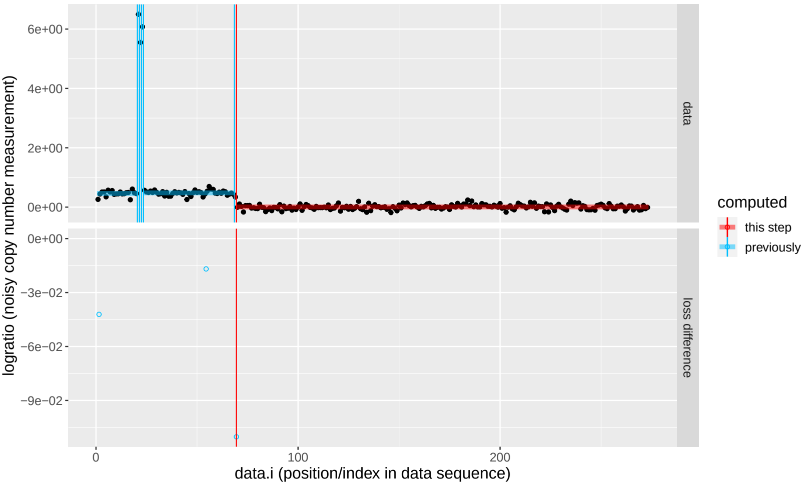
Visualization of computations at each iteration



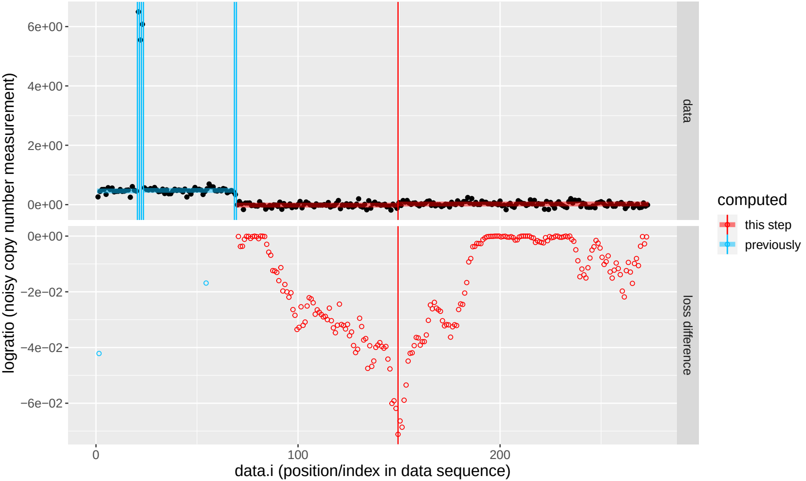
Visualization of computations at each iteration



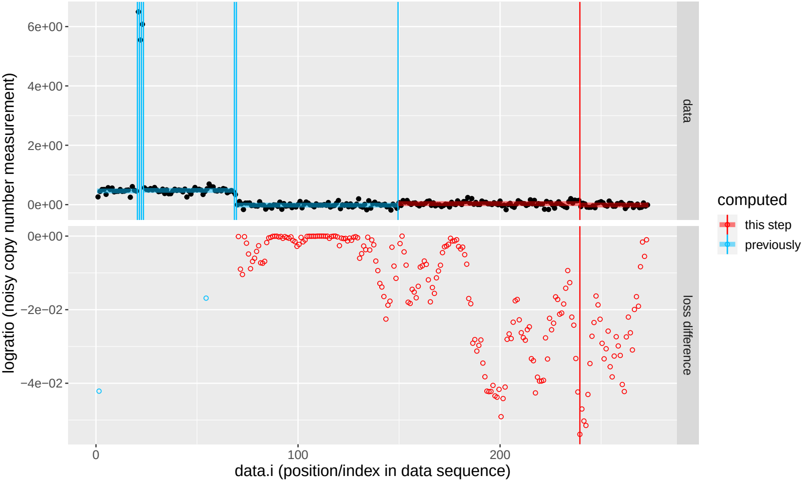
Visualization of computations at each iteration



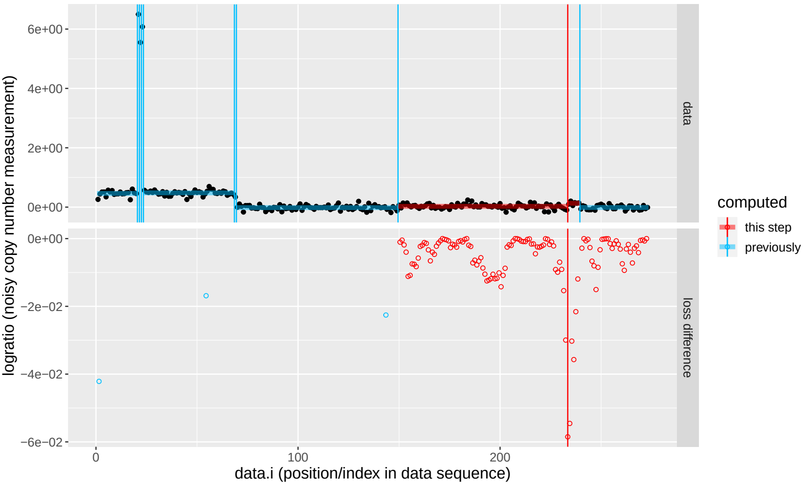
Visualization of computations at each iteration



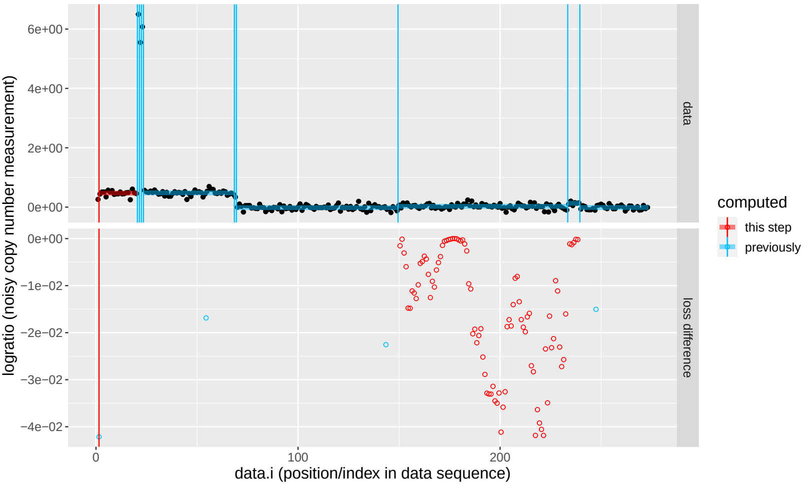
Visualization of computations at each iteration



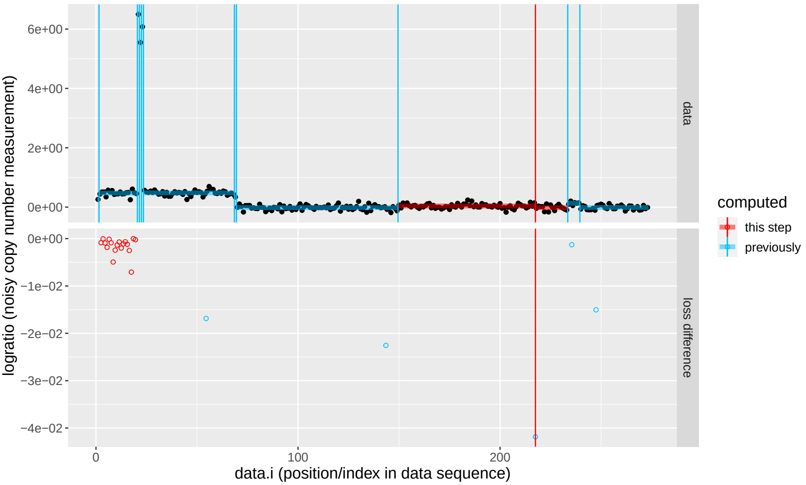
Visualization of computations at each iteration



Visualization of computations at each iteration



Visualization of computations at each iteration



Complexity analysis

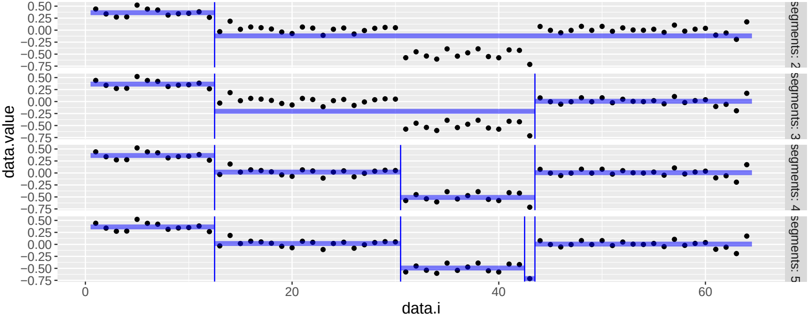
- Assume n data and K segments.
- Computing best loss decrease and split point for a segment with t data takes $O(t)$ time.
- Keep a list of segments which could be split, sorted by loss decrease values.
- Best case is when segments get cut in half each time, $O(n \log K)$ time. (minimize number of possible splits for which we have to recompute loss)
- Worst case is when splits are very unequal $(1, t-1)$, $O(nK)$ time. (maximize number of possible splits for which we have to recompute loss)

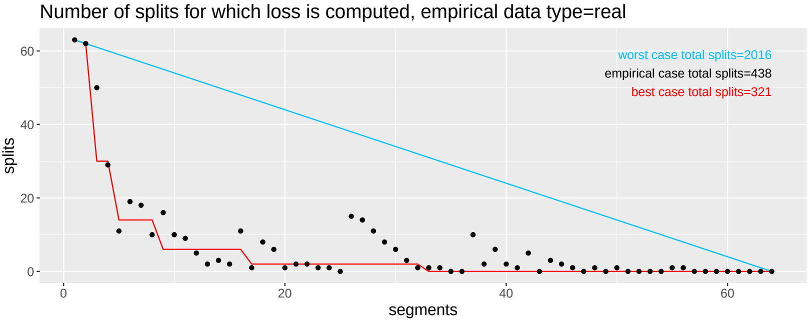
Detailed complexity analysis

- Let $n = 2^J$ for some $J \in \{1, 2, \dots\}$, for example $J = 6 \Rightarrow n = 64$.
- For any $j \in \{1, \dots, J+1\}$ if we do $I = 2^{j-1}$ iterations then how many split cost values to compute?
- Best case: $nj - 2^j + 1 = n(1 + \log_2 I) - I/2 + 1 \Rightarrow O(n \log I)$.
- Worst case: $nI - I(1+I)/2 \Rightarrow O(nI)$.

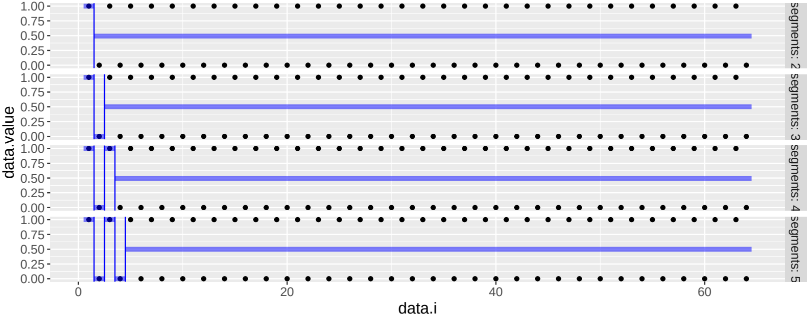
j	I	best	total	worst	total
1	1	$n - 1 = 63$	$n - 1 = 63$	$n - 1 = 63$	$n - 1 = 63$
2	2	$n - 2 = 62$	$2n - 3 = 125$	$n - 2 = 62$	$2n - 3 = 125$
	3	$n/2 - 2 = 30$		$n - 3 = 61$	$3n - 6 = 186$
3	4	$n/2 - 2 = 30$	$3n - 7 = 185$	$n - 4 = 60$	$4n - 10 = 246$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
4	8	$n/4 - 2 = 14$	$4n - 15 = 241$	$n - 8 = 56$	$8n - 36 = 476$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
7	64	$n/32 - 2 = 0$	$7n - 128 = 321$	$n - 64 = 0$	$64n - 2080 = 2016$

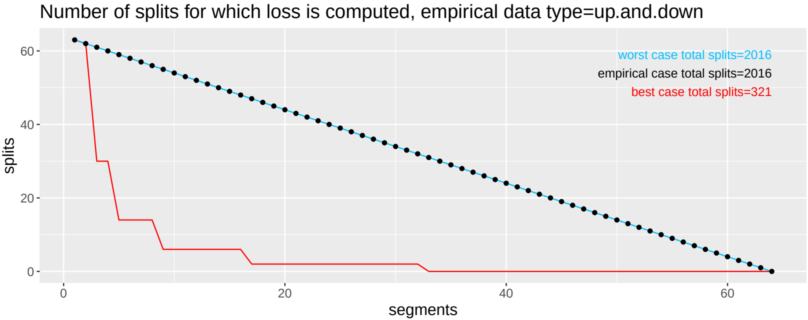
Real data time complexity analysis



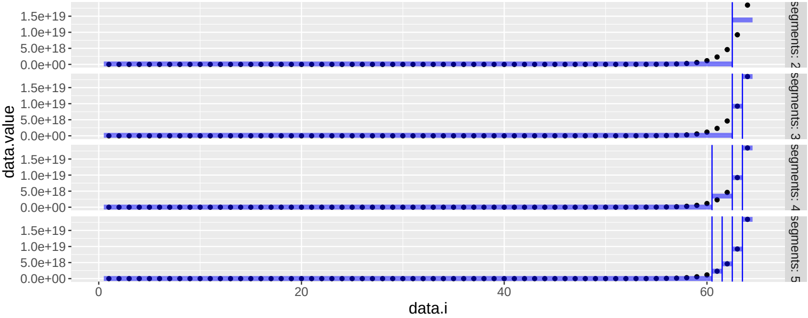


Synthetic data time complexity analysis

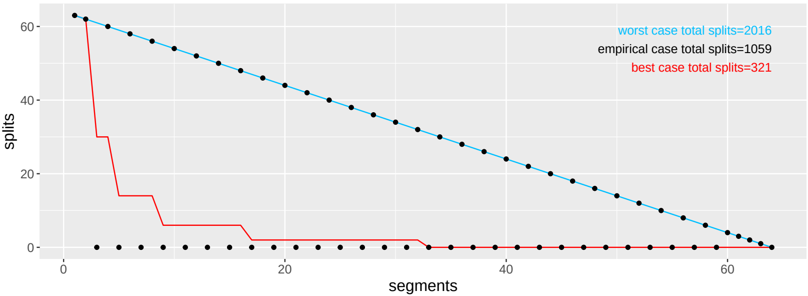




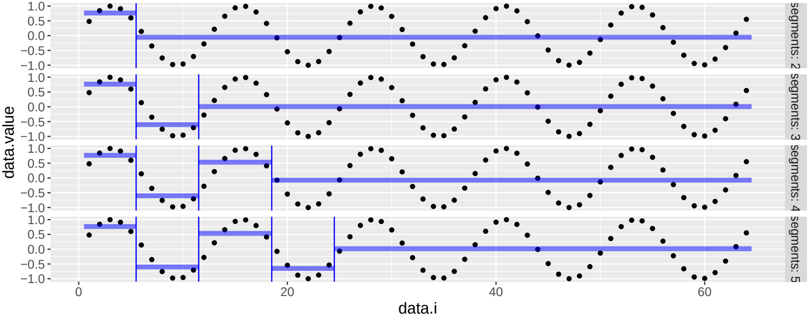
Synthetic data time complexity analysis

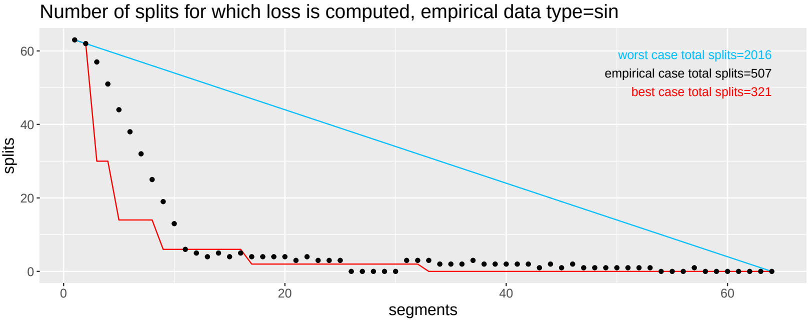


Number of splits for which loss is computed, empirical data type=exponential

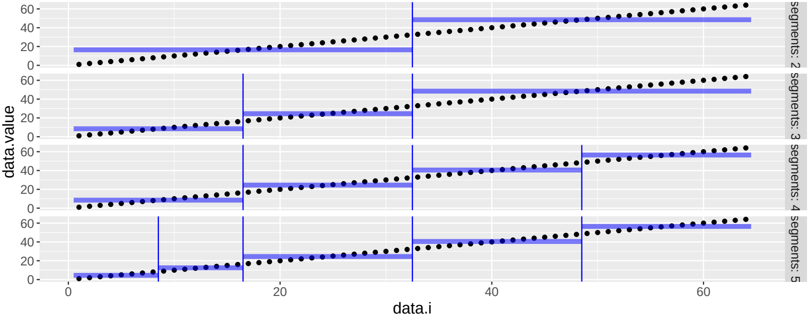


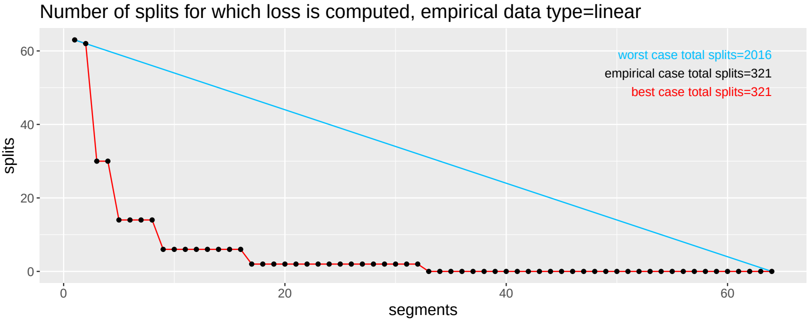
Synthetic data time complexity analysis





Synthetic data time complexity analysis





Analysis of insert time and storage

To store previously computed best loss/split for each segment, use a C++ Standard template library multimap, keyed by loss decrease. If multimap has p items then insert takes $O(\log p)$ time. Below: inserts column shows p for each insert, and size column shows p after inserts. Total $-\log(I-1) + \sum_{p=1}^{I-1} 2\log p \in O(I \log I)$ time over all inserts, smaller than $O(n \log I)$ time for split computation.

	equal splits		unequal splits	
iteration I	inserts	size	inserts	size
1	0	1	0	1
2	0,1	2	0	1
3	1,2	3	0	1
⋮	⋮	⋮	⋮	⋮
32	30,31	32	0	1
33		31	0	1
34		30	0	1
⋮	⋮	⋮	⋮	⋮
62		2	0	1
63		1	0	1

Comparison with previous algorithms from clustering

- Binary segmentation has segment/cluster-specific mean parameter, as in K-means and Gaussian mixture models. These algorithms attempt optimization of an error function which measures how well the means fit the data (but are not guaranteed to compute the globally optimal/best model).
- Binary segmentation is deterministic (different from K-means/GMM which requires random initialization). It performs a sequence of greedy minimizations (as in hierarchical clustering).
- Binary segmentation defines a sequence of split operations (from 1 segment to N segments), whereas agglomerative hierarchical clustering defines a sequence of join operations (from N clusters to 1 cluster). Data with common segment mean must be adjacent in time/space; hierarchical clustering joins may happen between any pair of data points (no space/time dimension).

Possible exam questions

- Explain in detail one similarity and one difference between binary segmentation and k-means. (gaussian mixture models, hierarchical clustering)
- For a sequence of $n = 10$ data, we need to compute the loss for each of the 9 possible splits in the first iteration of binary segmentation. What is the number of splits for which we must compute the loss in the second/third steps? (best and worst case)