

Why does functional pruning yield such fast algorithms for optimal changepoint detection?

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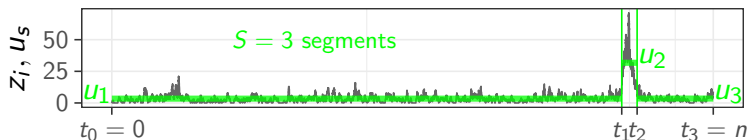
Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

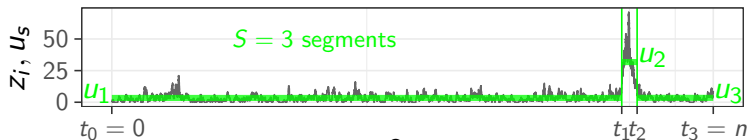
Theoretical time complexity

Statistical model is a piecewise constant mean



- ▶ We have n data $z_1, \dots, z_n \in \mathbb{Z}_+$.
- ▶ Fix the number of segments $S \in \{1, 2, \dots, n\}$.
- ▶ Optimization variables: $S - 1$ changepoints $t_1 < \dots < t_{S-1}$ and S segment means $u_1, \dots, u_S \in \mathbb{R}_+$.
- ▶ Let $0 = t_0 < t_1 < \dots < t_{S-1} < t_S = n$ be the segment limits.
- ▶ Statistical model: for every segment $s \in \{1, \dots, S\}$, $z_i \stackrel{\text{iid}}{\sim} \text{Poisson}(u_s)$ for every data point $i \in (t_{s-1}, t_s]$ implies convex loss function $\ell(u, z) = u - z \log u$ to minimize.
- ▶ Other models: real-valued $z_i \stackrel{\text{iid}}{\sim} N(u_s, \sigma^2)$ implies square loss $\ell(u, z) = (u - z)^2$, etc.

Maximum likelihood inference is a non-convex minimization problem

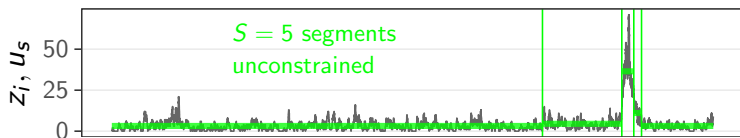


$$\begin{aligned}\mathcal{L}_{S,n} &= \min_{\substack{\mathbf{u} \in \mathbb{R}^S \\ 0=t_0 < t_1 < \dots < t_{S-1} < t_S=n}} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i) \\ &= \underbrace{\min_{t_{S-1}} \min_{\substack{u_1, \dots, u_{S-1} \\ t_1 < \dots < t_{S-2}}} \sum_{s=1}^{S-1} \sum_{i=t_{s-1}+1}^{t_s}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

- ▶ Hard optimization problem, naively $O(n^S)$ time.
- ▶ Auger and Lawrence (1989): $O(Sn^2)$ time classical dynamic programming algorithm:

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

Maximum likelihood inference is a non-convex minimization problem



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Efficient computation of optimal last segment cost

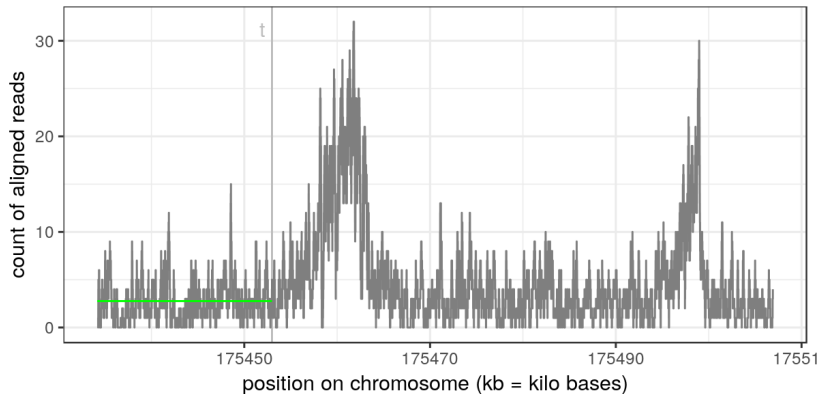
For any $0 \leq i < j \leq n$ we have

$$\begin{aligned}c_{(i,j]} &= \min_u \sum_{t=i+1}^j (u - z_t)^2 \\&= \min_u \sum_{t=i+1}^j (u^2 - 2uz_t + z_t^2) \\&= \sum_{t=i+1}^j (z_t^2) + \min_u (j-i)u^2 - 2u \sum_{t=i+1}^j (z_t) \\&= Q_j - Q_i + (S_j - S_i)^2/(j-i) - 2(S_j - S_i)/(j-i) \\&= Q_j - Q_i - (S_j - S_i)^2/(j-i)\end{aligned}$$

where

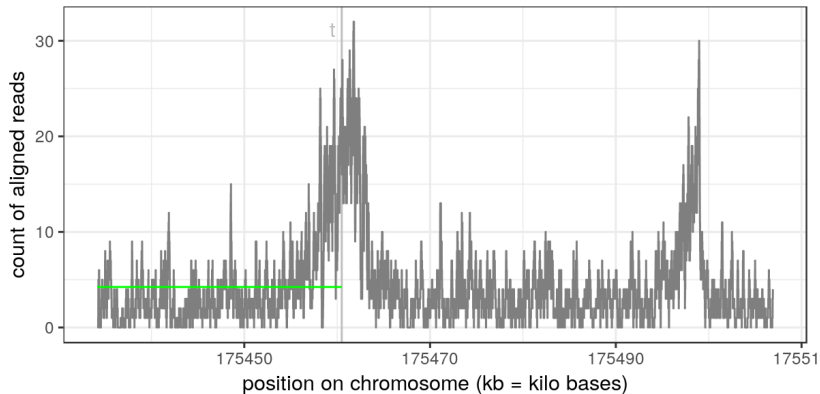
- ▶ $Q_0 = 0$ and $Q_i = Q_{i-1} + z_i^2$ for all $i \in \{1, \dots, n\}$ (cumulative sum of squares of data).
- ▶ $S_0 = 0$ and $S_i = S_{i-1} + z_i$ for all $i \in \{1, \dots, n\}$ (cumulative sum of data).

Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 1$ segments up to data point t



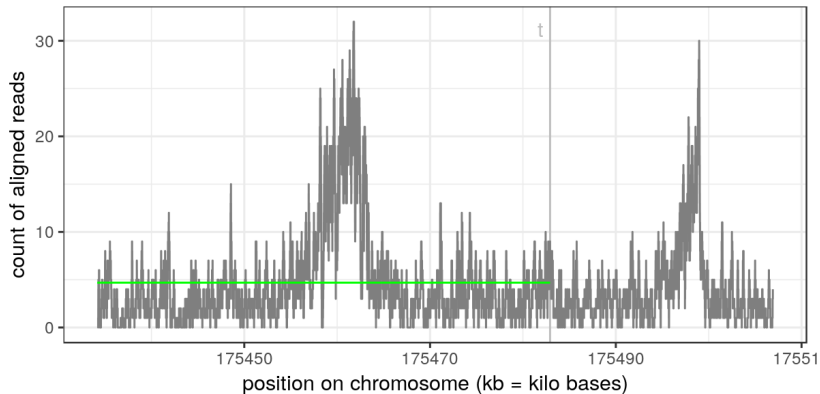
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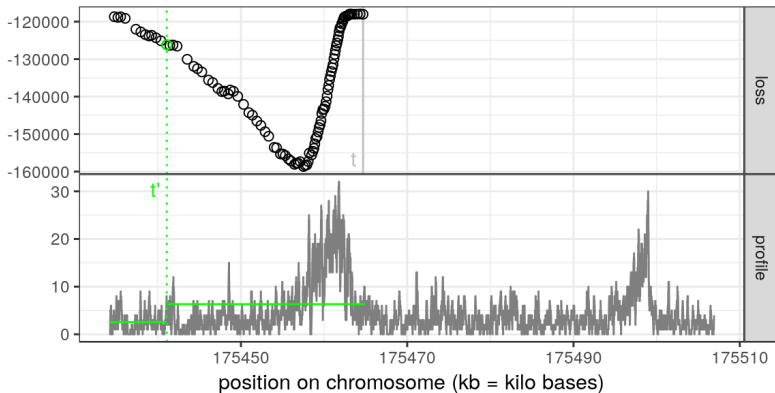
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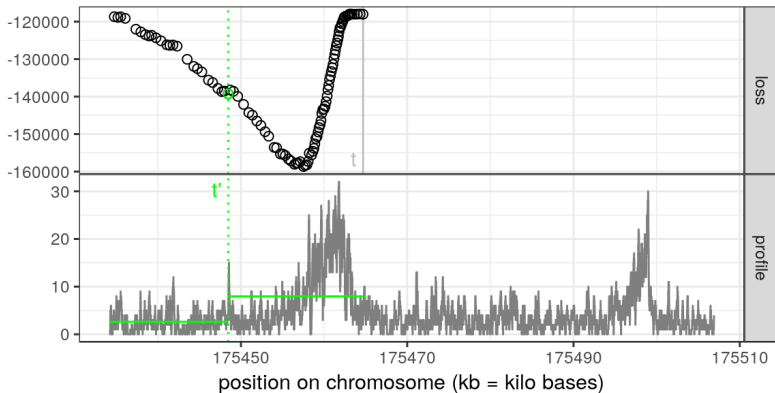
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Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 2$ segments up to data point $t < d$



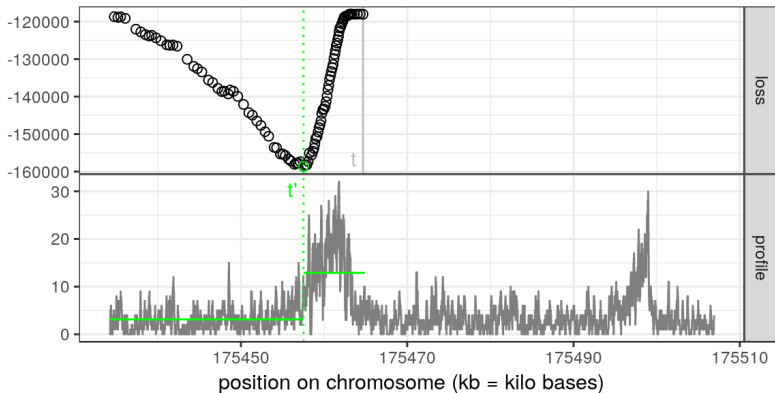
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 2$ segments up to data point $t < d$



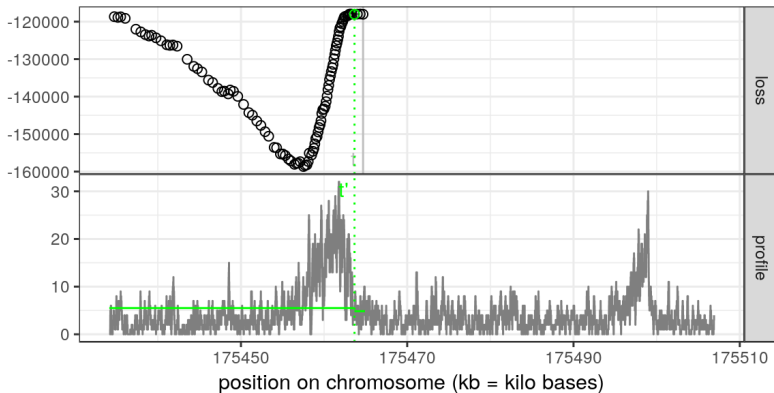
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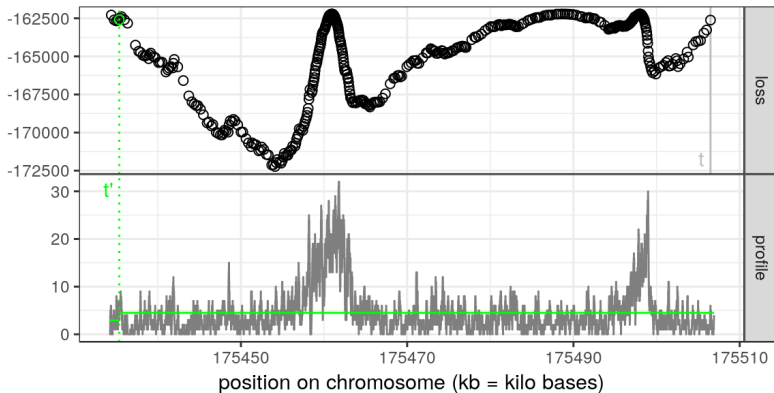
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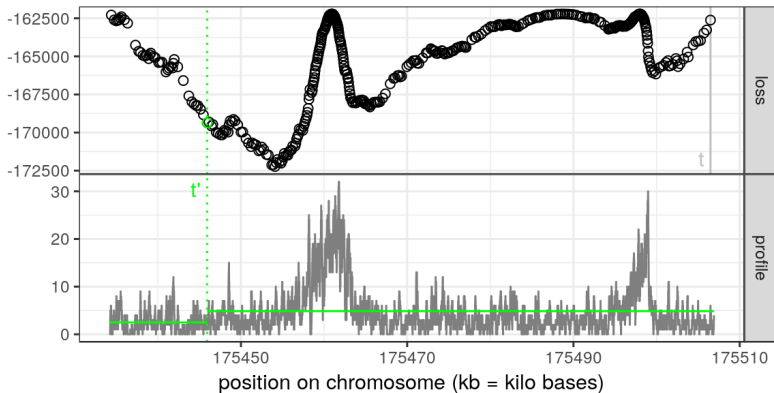
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Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 2$ segments up to last data point $t = d$



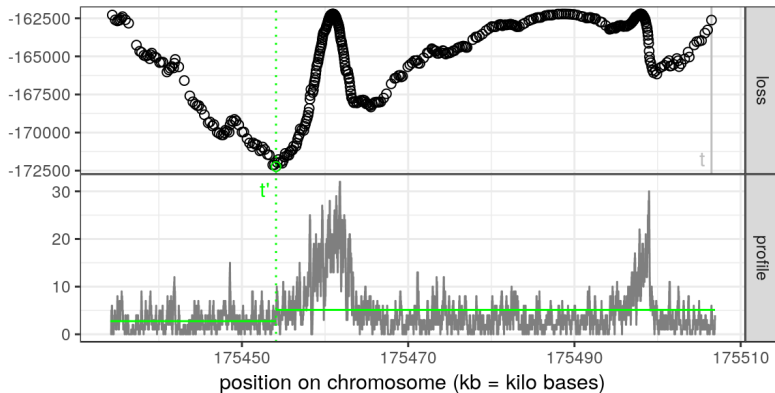
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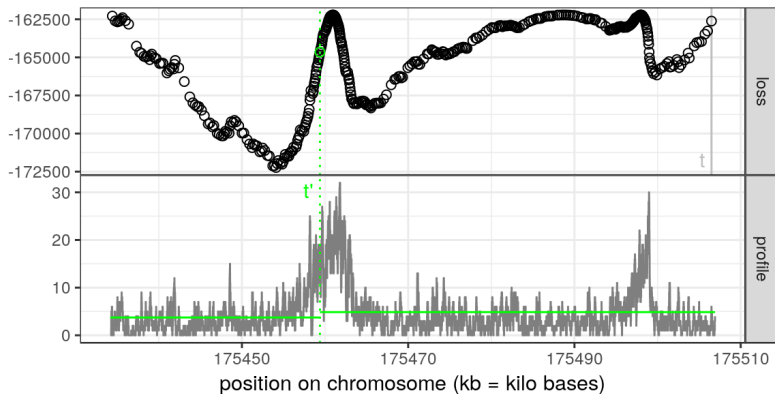
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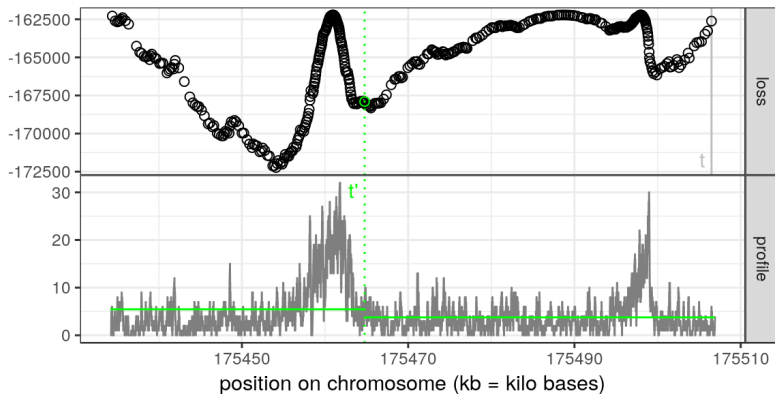
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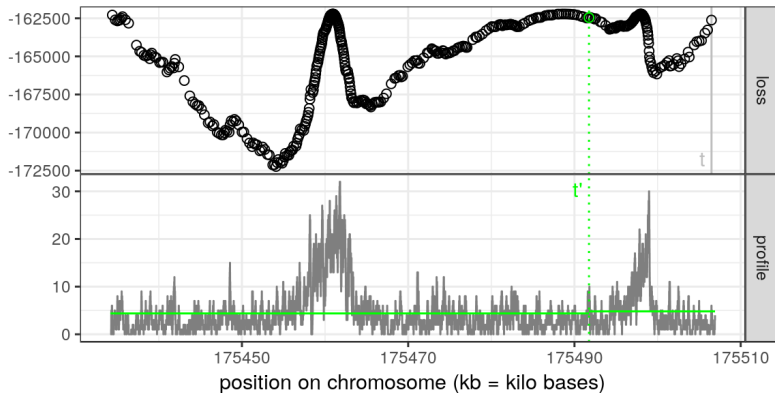
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Dynamic programming is faster than grid search for $s > 2$ segments

Computation time in number of data points n :

segments s	grid search	dynamic programming
1	$O(n)$	$O(n)$
2	$O(n^2)$	$O(n^2)$
3	$O(n^3)$	$O(n^2)$
4	$O(n^4)$	$O(n^2)$
\vdots	\vdots	\vdots

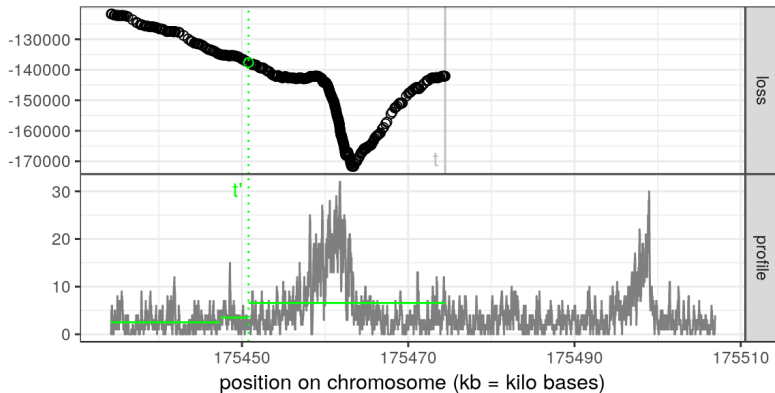
For example $n = 5735$ data points to segment.

$$n^2 = 32890225$$

$$n^3 = 188625440375$$

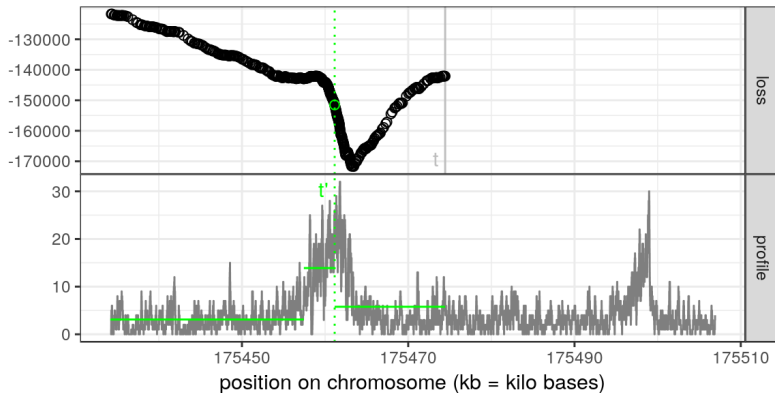
\vdots

Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 3$ segments up to data point t



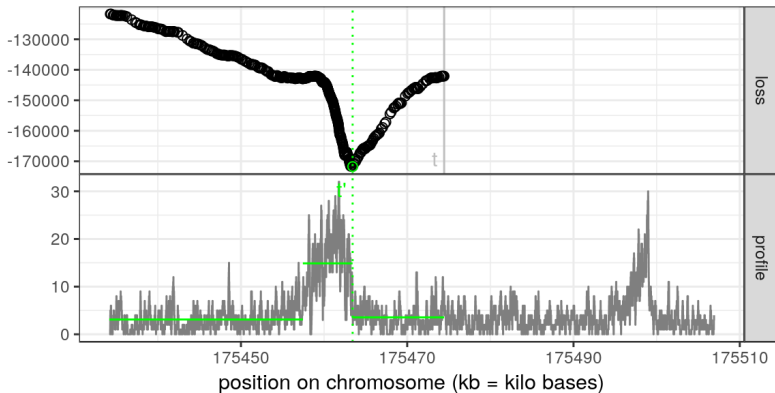
$$\mathcal{L}_{3,t} = \min_{t' < t} \underbrace{\mathcal{L}_{2,t'}}_{\text{optimal loss in 2 segments up to } t'} + \underbrace{C_{(t',t]}}_{\text{optimal loss of 3rd segment } (t', t]}$$

Computation of optimal loss $\mathcal{L}_{s,t}$ for $s = 3$ segments up to data point t



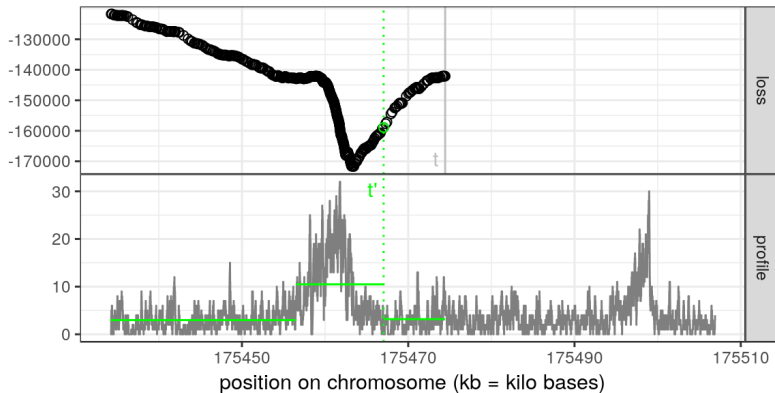
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Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

Theoretical time complexity

Classical dynamic programming is too slow for big data

- ▶ Motivated by big data sequences $n > 1000$ in genomics and other fields, for which $O(n^2)$ is too slow.
- ▶ Recent work into functional pruning algorithms which compute the same solution in $O(n \log n)$ (empirically).
- ▶ Independent discovery by Rigaiil arXiv:1004.0887, JFdS 2015; Johnson PhD 2011, JCGS 2013. Main idea: first minimize on the last changepoint t_{S-1} , then on the last segment mean u_S :

$$\begin{aligned}\mathcal{L}_{S,n} &= \min_{t_{S-1}} \mathcal{L}_{S-1,t_{S-1}} + \underbrace{\min_{u_S} \sum_{i=t_{S-1}+1}^{t_S=n} \ell(u_S, z_i)}_{C_{(t_{S-1}, t_S=n]}} \text{ — classical} \\ &= \underbrace{\min_{u_S} \min_{t_{S-1}} \mathcal{L}_{S-1,t_{S-1}}}_{C_{S,n}(u_S)} + \sum_{i=t_{S-1}+1}^{t_S=n} \ell(u_S, z_i) \text{ — functional}\end{aligned}$$

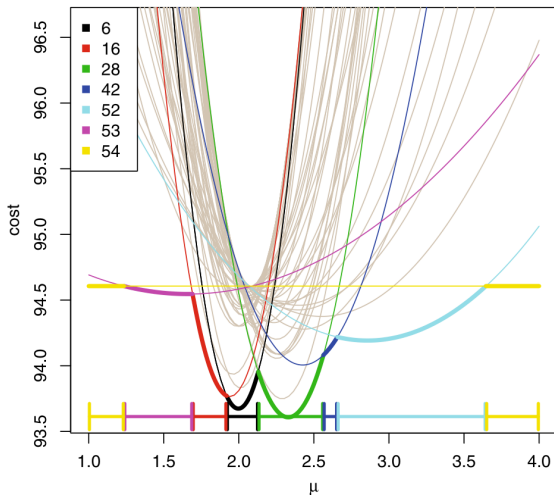
Dynamic programming recursion with functional pruning

- ▶ τ is first data point on last segment.
- ▶ μ is last segment mean.

$$\begin{aligned}C_{S,n}(\mu) &= \min_{\tau \in \{S, \dots, n\}} \mathcal{L}_{S-1, \tau-1} + \sum_{i=\tau}^n \ell(\mu, z_i) \\&= \min \left\{ \mathcal{L}_{S-1, S-1} + \sum_{i=S}^n \ell(\mu, z_i), \dots, \right. \\&\quad \left. \mathcal{L}_{S-1, n-1} + \ell(\mu, z_n) \right\} \\&= \ell(\mu, z_n) + \min \left\{ \mathcal{L}_{S-1, S-1} + \sum_{i=S}^{n-1} \ell(\mu, z_i), \dots, \right. \\&\quad \left. \mathcal{L}_{S-1, n-2} + \ell(\mu, z_{n-1}) \right\} \\&\quad \left. \mathcal{L}_{S-1, n-1} \right\} \\&= \ell(\mu, z_n) + \min \{ C_{S, n-1}(\mu), \mathcal{L}_{S-1, n-1} \}\end{aligned}$$

Functional cost representation results in pruning

Maidstone, *et al.* Statistics and Computing 2016.



- ▶ Only need to store the minimum cost (colored lines/intervals).
- ▶ No need to consider the cost functions/changepoints which are not optimal for any mean values (grey lines).

Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

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Number of intervals in real and simulated data

Rigaill, arXiv:1004.0887.

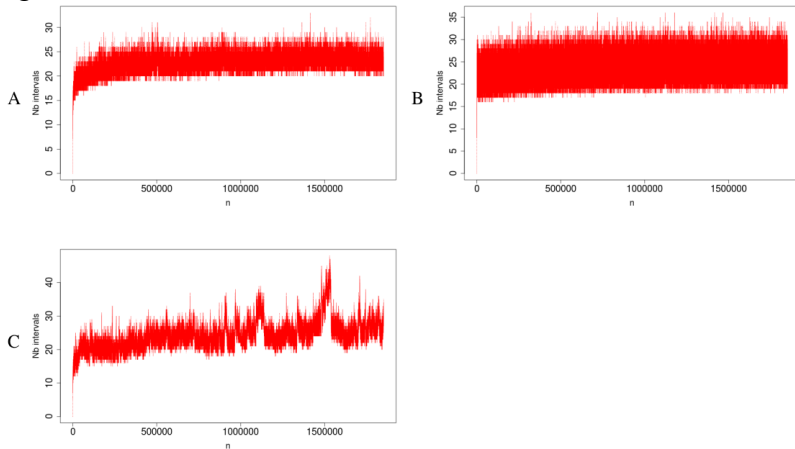
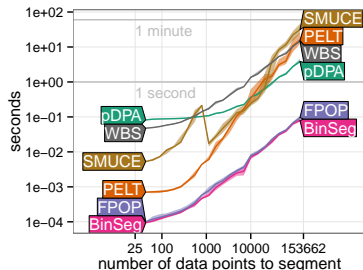
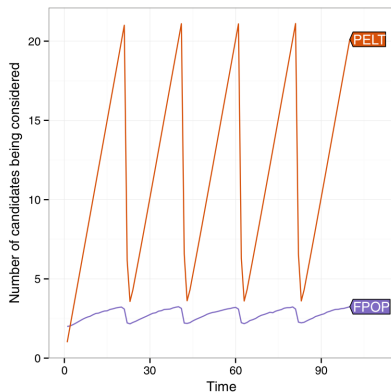


FIGURE 5. Maximum number of intervals stored by the pDPA at each point of the sequence for $K = 1$. A: For 100 sequences of $1.8 \cdot 10^6$ points simulated with a constant signal plus an additional normal noise of variance 1. B: For 100 sequences of $1.8 \cdot 10^6$ points simulated with a sine wave signal plus an additional normal noise of variance 1. C: For the 18 profiles of length $1.8 \cdot 10^6$ of the GSE17359 dataset.

Another fast functional pruning algorithm

Maidstone, *et al.* Statistics and Computing 2016.

$$\underset{\mathbf{m} \in \mathbb{R}^n}{\text{minimize}} \quad \sum_{i=1}^n \ell(m_i, z_i) + \lambda \sum_{i=1}^{n-1} I[m_i \neq m_{i+1}]$$



Algorithm with constraints is also fast

H, et al. arXiv:1703.03352.

$$\begin{aligned} & \underset{\mathbf{m} \in \mathbb{R}^n}{\text{minimize}} && \sum_{i=1}^n \ell(m_i, z_i) \\ & \text{subject to} && \sum_{i=1}^{n-1} I[m_i \neq m_{i+1}] = S - 1, \\ & && \text{...up-down constraints on } m. \end{aligned}$$

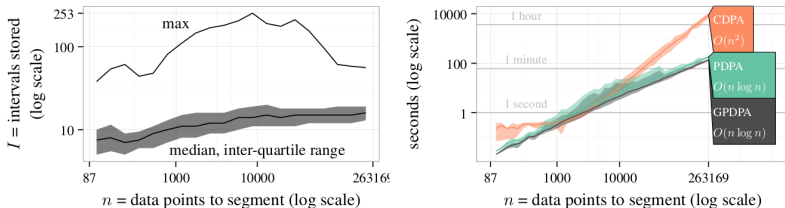
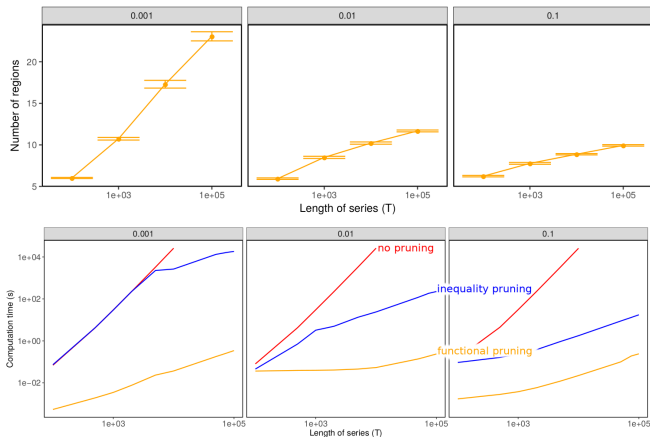


Figure 3: Empirical speed analysis on 2752 count data vectors from the histone mark ChIP-seq benchmark. For each vector we ran the GPDPA with the up-down constraint and a max of $K = 19$ segments. The expected time complexity is $O(KnI)$ where I is the average number of intervals (function pieces; candidate changepoints) stored in the $C_{k,t}$ cost functions. **Left:** number of intervals stored is $I = O(\log n)$ (median, inter-quartile range, and maximum over all data points t and segments k). **Right:** time complexity of the GPDPA is $O(n \log n)$ (median line and min/max band).

Another fast constrained algorithm for neuroscience

Jewell, et al. *Biostatistics* 2019.

$$\begin{aligned} & \underset{c_1, \dots, c_T, z_2, \dots, z_T}{\text{minimize}} && \frac{1}{2} \sum_{t=1}^T (y_t - c_t)^2 + \lambda \sum_{t=2}^T 1_{(z_t \neq 0)} \\ & \text{subject to} && z_t = c_t - \gamma c_{t-1} \geq 0. \end{aligned}$$

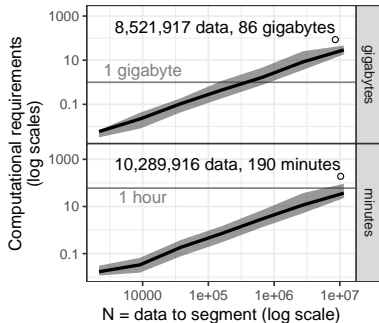
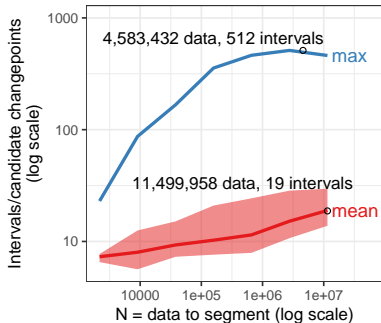


Another fast constrained algorithm for genomics

H, et al. arXiv:1810.00117, accepted in *J. Statistical Software*.

$$\underset{\mathbf{m} \in \mathbb{R}^n}{\text{minimize}} \quad \sum_{i=1}^n \ell(m_i, z_i) + \lambda \sum_{i=1}^{n-1} I[m_i \neq m_{i+1}]$$

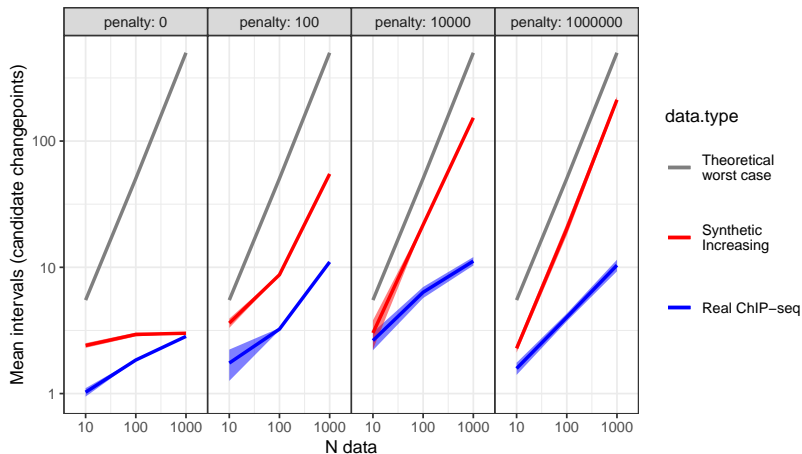
subject to ...up-down constraints on m .



$I = O(\log n)$ intervals.

Overall $O(n \log n)$ complexity.

Worst case quadratic complexity only observed with synthetic data and large penalties



Mean \pm standard deviation over 10 data sets.

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Theoretical time complexity

Worst case complexity is quadratic

Rigaill, arXiv:1004.0887.

Proposition 5. *If all $\sum_j \gamma(Y_j, \mu)$ are unimodal in μ and if both minimising $\tilde{C}_{1:t, \tau}^K(\mu)$ and finding the roots of $\tilde{C}_{1:t, \tau}^K(\mu) = \mathbf{Cost}_{1:t}^{K-1}$ are in $\mathcal{O}(1)$, the pDPA is at worst in $\mathcal{O}(K_{\max} n^2)$ time and in $\mathcal{O}(K_{\max} n)$ space.*

Proof. The key quantity to control is the number of intervals needed to represent $\mathcal{S}_{1:t, \tau}^K$. For a given K and at step t the number of candidate last change-points is obviously bounded by t . If all $\sum_{j=\tau+1}^{t+1} \gamma(Y_j, \mu)$ are unimodal, using theorem 8 (proved in appendix A) we get that the total number of intervals is bounded by $2t - 1$. Thus at each step there is at most t last change-points and $2t - 1$ intervals to update. By summing all these bounds from 1 to n and for every possible K we retrieve an $\mathcal{O}(K_{\max} n^2)$ worst case time complexity.

As for the worst case space complexity, we need to store two $(n + 1) \times K_{\max}$ matrices ($D_{K,t}$ and $I_{K,t}$) and at each step there is at most t candidates and $2t - 1$ intervals. This gives an $\mathcal{O}(K_{\max} n)$ space complexity ■

Average case complexity proof for uniform loss

Rigaill, arXiv:1004.0887.

Property 6. *For the negative log-likelihood loss, $K_{max} = 1$, and for, $Y_{1:n+1}$, n independent and identically distributed random variables of density f and continuous distribution F , $E(|\tau_{1:n}^1|) = \mathcal{O}(\log(n))$ and the average time complexity of the pDPA is in $\mathcal{O}(n\log(n))$.*

Proof The proof of $E(|\tau_{1:t}^1|) = \mathcal{O}(\log(t))$ is given in appendix B. We obtain this result by studying the set $\mathcal{S}_{1:n,\tau}^1$. More precisely we characterize some simple events for which $\mathcal{S}_{1:n,\tau}^1$ is empty and compute the probability of these events. Then by taking the expectation and summing over all possible τ we get the desired result.

For the complexity using theorem 8 we know that the number of intervals stored by the pruned DPA is always smaller than 2 times the number of candidate change-points. Thus for $K_{max} = 1$, for every $t \leq n$ the pruned DPA updates on average $\mathcal{O}(\log(t))$ functional costs and intervals. From this the complexity follows ■

Conclusions

- ▶ Optimal detection of $S - 1$ changepoints in n data is naively a $O(n^S)$ computation.
- ▶ Functional pruning method yields algorithms with worst case time complexity of $O(n^2)$ (same as classical dynamic programming).
- ▶ Empirically the functional pruning algorithms are much faster, $O(n \log n)$.
- ▶ Only one proof of average time complexity for 1 changepoint and the uniform loss function (never used in practice).
- ▶ Would be interesting to prove $O(n \log n)$ average time complexity in other more realistic situations. (square/Poisson loss, λ) How?
- ▶ Let's collaborate! toby.hocking@nau.edu

Example data set with $n = 4$

Rigaill, arXiv:1004.0887.

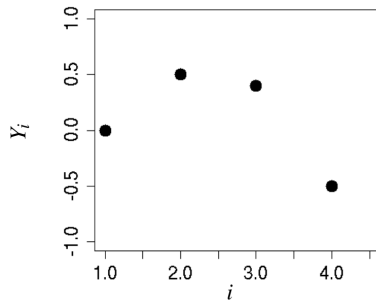
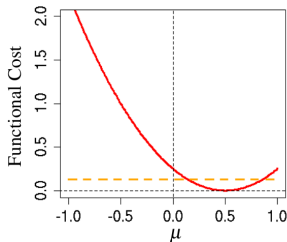


FIGURE 1. *Four-point signal. y_i as a function of i . $y_1 = 0$, $y_2 = 0.5$, $y_3 = 0.4$, $y_4 = -0.5$*

Functional cost computation at $t = 3$

Rigaill, arXiv:1004.0887.

- ▶ Data: 0, 0.5, 0.4, -0.5.
- ▶ $\mathcal{L}_{1,1} = \min_{\mu}(\mu - 0)^2 = 0$.
- ▶ $\mathcal{L}_{1,2} = \min_{\mu}(\mu - 0)^2 + (\mu - 0.5)^2 = 0.125$.
- ▶ Computing $C_{2,3}(\mu) = \ell(\mu, z_3) + \min\{C_{2,2}(\mu), \mathcal{L}_{1,2}\}$:
- ▶ Change before $\tau = 2$: $C_{2,2}(\mu) = \mathcal{L}_{1,1} + (\mu - 0.5)^2$.
- ▶ Change before $\tau = 3$: $\mathcal{L}_{1,2}$.



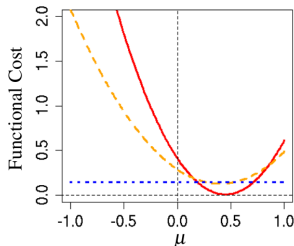
τ	Functional cost	$\mathcal{S}_{1:3,\tau}^1$
2	$0.25 - \mu + \mu^2$	$[0.146, 0.854]$
3	0.125	$[-\infty, 0.146] \cup [0.854, +\infty]$

FIGURE 2. Functional cost of $Y_{1:3}$ for $K = 1$ using the quadratic loss. (Left) Functional cost as a function of μ of segmentations having a change-point at $\tau = 2$ (solid red) and $\tau = 3$ (orange dashed). (Right) Analytical expression of the functional costs for $\tau = 2$ and $\tau = 3$ and the set of μ , for which they are optimal: $\mathcal{S}_{1:3,\tau}^1$.

Functional cost computation at $t = 4$

Rigaill, arXiv:1004.0887.

- ▶ Data: 0, 0.5, 0.4, -0.5.
- ▶ Computing $C_{2,4}(\mu) = \ell(\mu, z_4) + \min\{C_{2,3}(\mu), \mathcal{L}_{1,3}\}$:
- ▶ Change before $\tau = 2$: $\mathcal{L}_{1,1} + (\mu - 0.5)^2 + (\mu - 0.4)^2$.
- ▶ Change before $\tau = 3$: $\mathcal{L}_{1,2} + (\mu - 0.4)^2$.
- ▶ Change before $\tau = 4$:
 $\mathcal{L}_{1,3} = \min_{\mu}(\mu - 0)^2 + (\mu - 0.5)^2 + (\mu - 0.4)^2$.

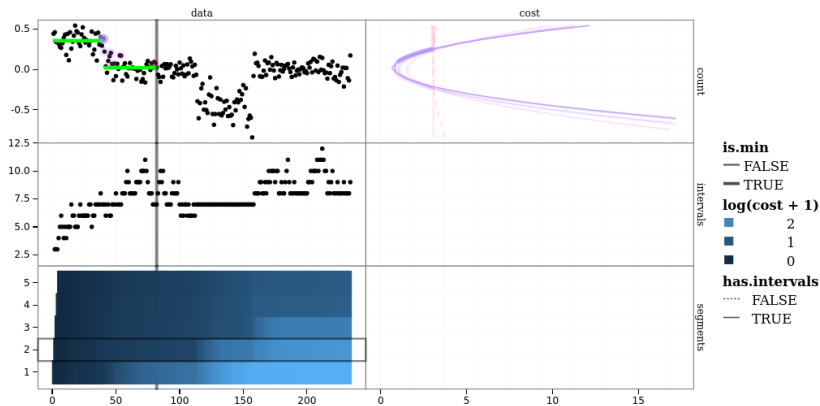


τ	Functional cost	$\mathcal{S}_{1:4,\tau}^1$
2	$0.41 - 1.8\mu + 2\mu^2$	$[0.190, 0.709]$
3	$0.285 - 0.8\mu + \mu^2$	\emptyset
4	0.14	$[-\infty, 0.190] \cup [0.709, +\infty]$

FIGURE 3. Functional cost of $Y_{1:4}$ for $K = 1$ using the quadratic loss. (Left) Functional cost of a segmentations having a change-point at $\tau = 2$ (solid red) $\tau = 3$ (orange dashed) and $\tau = 4$ (blue dotted). (Right) Analytical expression of the functional costs for $\tau = 2, 3$ and 4 and the set of μ , for which they are optimal: $\mathcal{S}_{1:4,\tau}^1$.

Functional pruning larger example

- ▶ Computing each $C_{s,t}(\mu)$ is an $O(I)$ operation where I is the number of intervals (candidate changepoints).
- ▶ Need to compute $O(Sn)$ functions; total complexity is $O(SnI)$.
- ▶ Empirically $I = O(\log n)$ due to pruning so overall $O(Sn \log n)$.



<http://members.cbio.mines-paristech.fr/~thocking/figure-unconstrained-PDPA-normal-big/>