

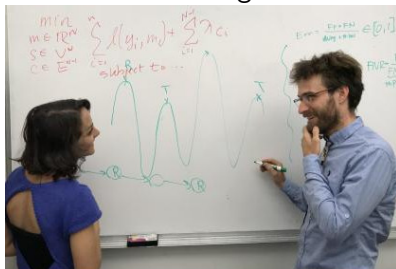
Why does functional pruning yield such fast algorithms for optimal changepoint detection?

Toby Dylan Hocking — toby.hocking@nau.edu

Northern Arizona University

School of Informatics, Computing, and Cyber Systems

Machine Learning Research Lab — <http://ml.nau.edu>



Come to Flagstaff! Graduate Research Assistantships available!

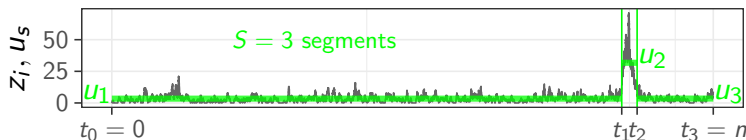
Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

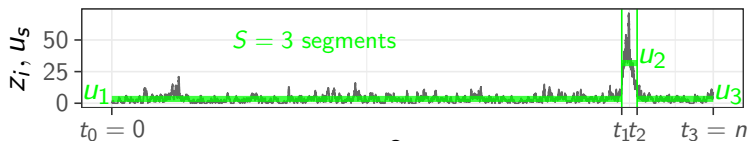
Theoretical time complexity

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 for S segments and n data is a non-convex minimization problem

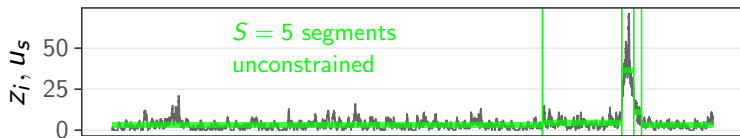


$$\begin{aligned}\mathcal{L}_{S,n} &= \min_{\substack{\mathbf{u} \in \mathbb{R}^S \\ 0=t_0 < t_1 < \dots < t_{S-1} < t_S=n}} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i) \\ &= \underbrace{\min_{t_{S-1}} \min_{\substack{u_1, \dots, u_{S-1} \\ t_1 < \dots < t_{S-2}}} \sum_{s=1}^{S-1} \sum_{i=t_{s-1}+1}^{t_s}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

- ▶ 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 for S segments and n data is a non-convex minimization problem

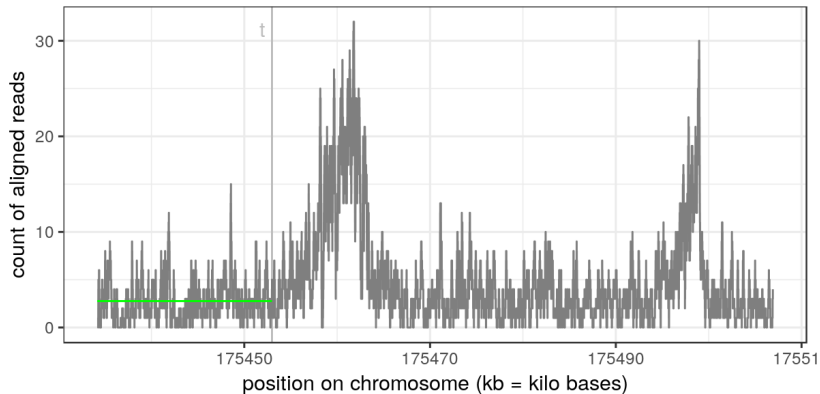


$$\begin{aligned}
 \mathcal{L}_{S,n} &= \min_{\mathbf{u} \in \mathbb{R}^S} \sum_{s=1}^S \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i) \\
 &= \min_{t_{S-1}} \underbrace{\min_{\substack{u_1, \dots, u_{S-1} \\ t_1 < \dots < t_{S-2}}} \sum_{s=1}^{S-1} \sum_{i=t_{s-1}+1}^{t_s} \ell(u_s, z_i)}_{\mathcal{L}_{S-1,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

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

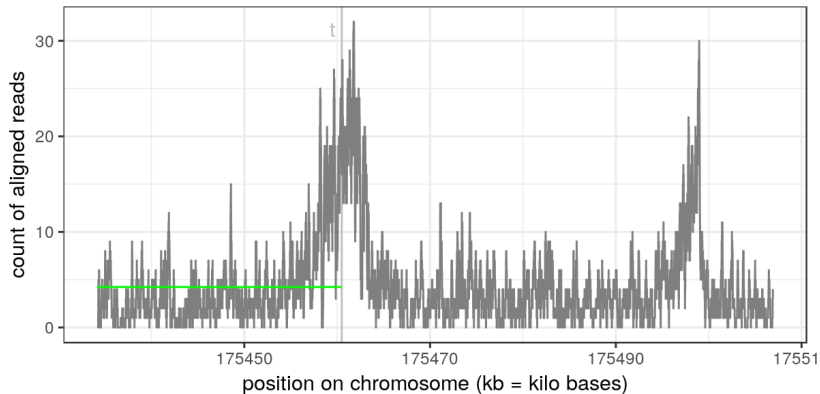
$$\mathcal{L}_{s,t} = \min_{t' < t} \mathcal{L}_{s-1,t'} + c_{(t',t]}$$

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



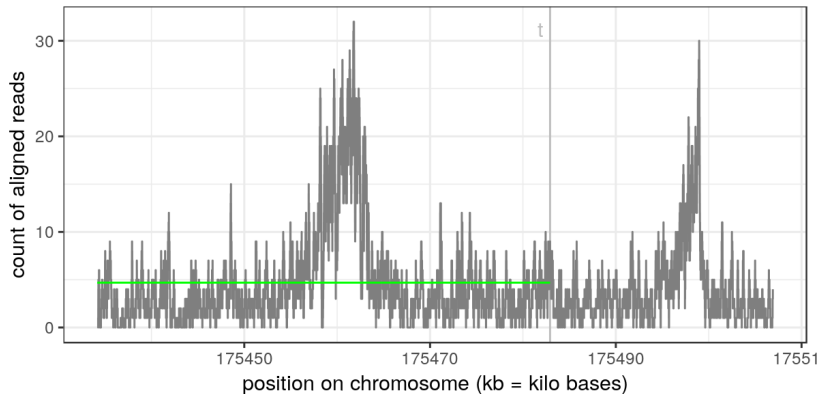
$$\mathcal{L}_{1,t} = \underbrace{c_{(0,t]}}_{\text{optimal loss of 1st segment } (0, t]}$$

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



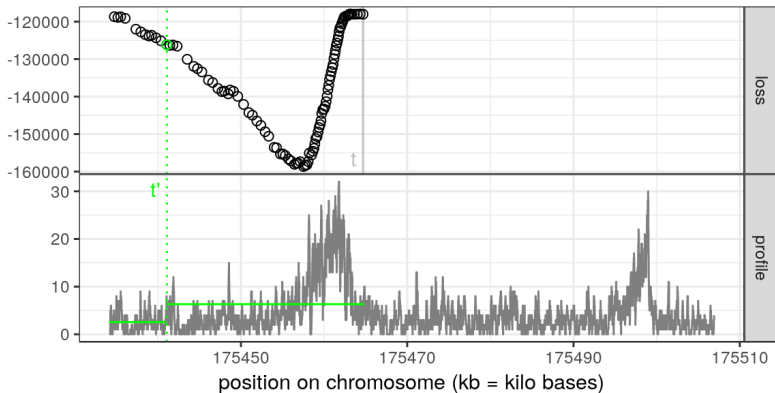
$$\mathcal{L}_{1,t} = \underbrace{C_{(0,t]}}_{\text{optimal loss of 1st segment } (0, t]}$$

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



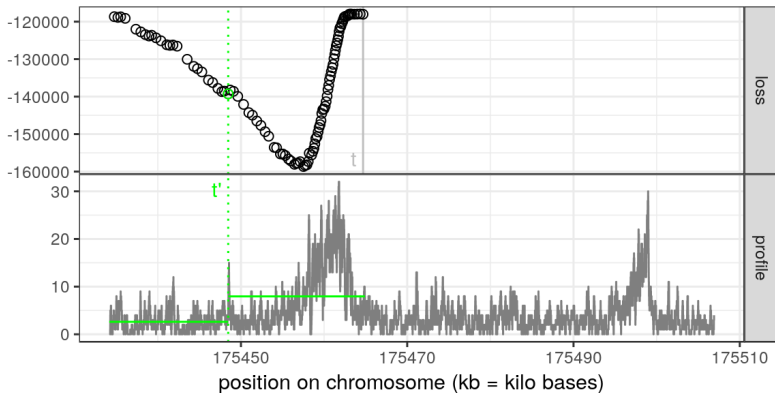
$$\mathcal{L}_{1,t} = \underbrace{c_{(0,t]}}_{\text{optimal loss of 1st segment } (0, t]}$$

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



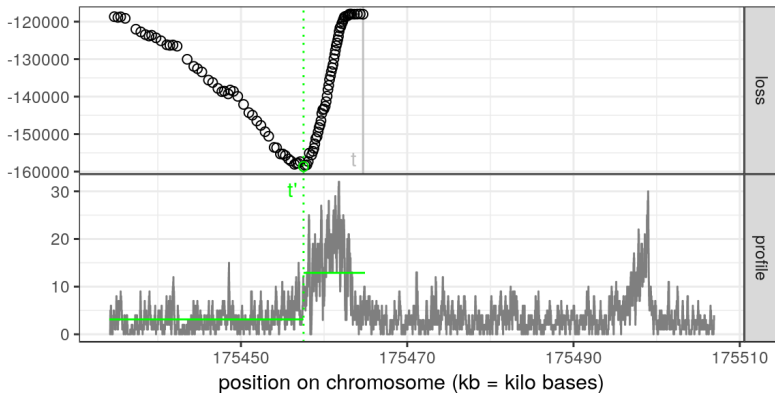
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



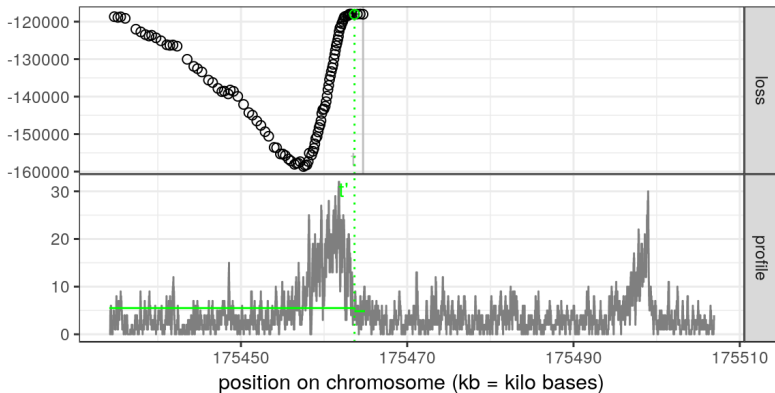
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



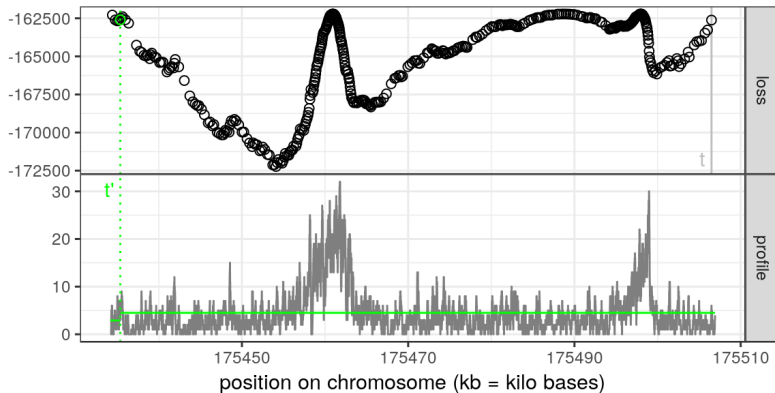
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



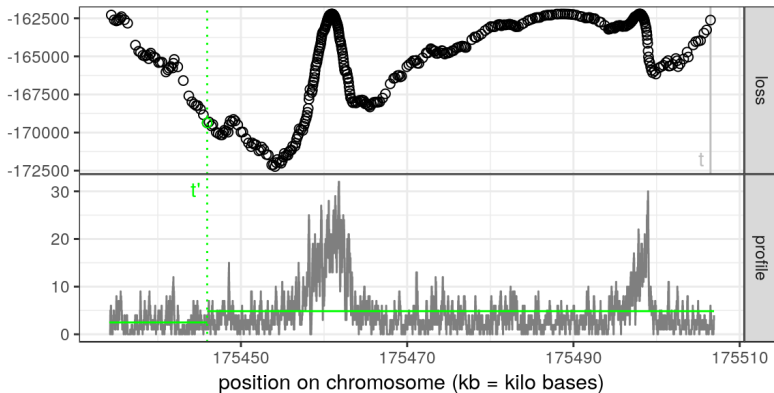
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



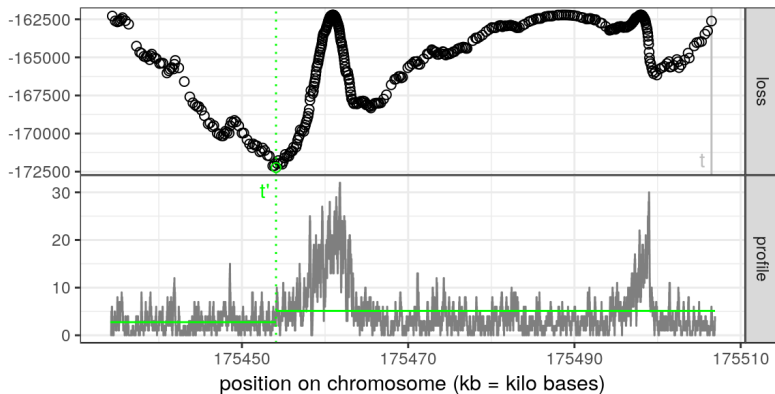
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



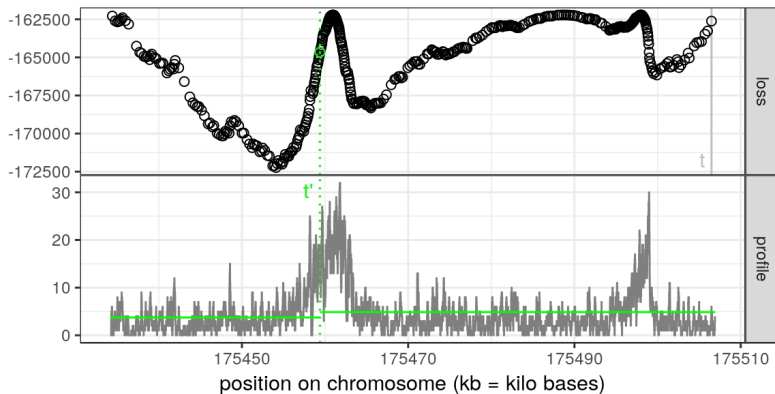
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



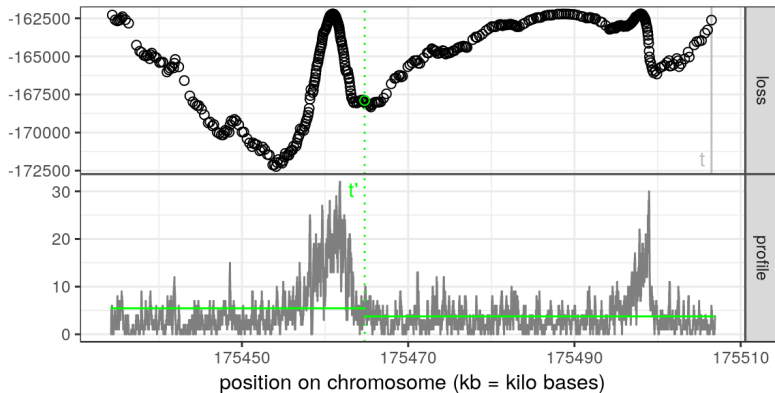
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



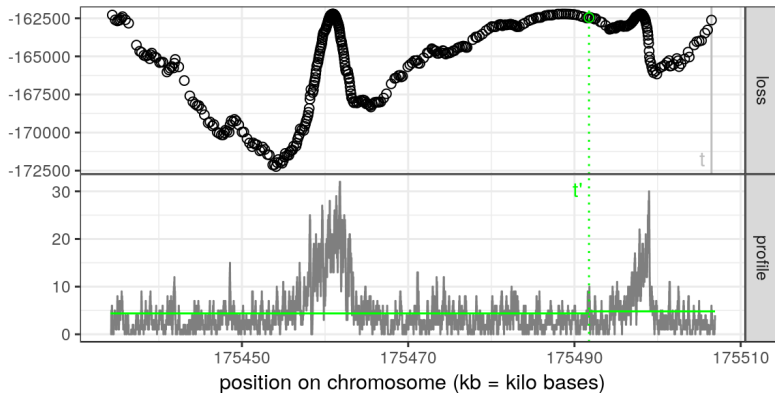
$$\mathcal{L}_{2,t} = \min_{t' < t} \underbrace{\mathcal{L}_{1,t'}}_{\text{optimal loss in 1 segment up to } t'} + \underbrace{C(t', t]}_{\text{optimal loss of 2nd segment } (t', t]}$$

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



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

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

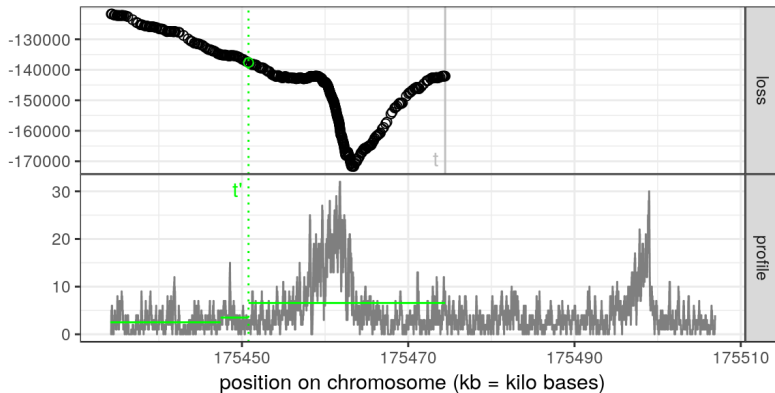
For example $n = 5735$ data points to segment.

$$n^2 = 32890225$$

$$n^3 = 188625440375$$

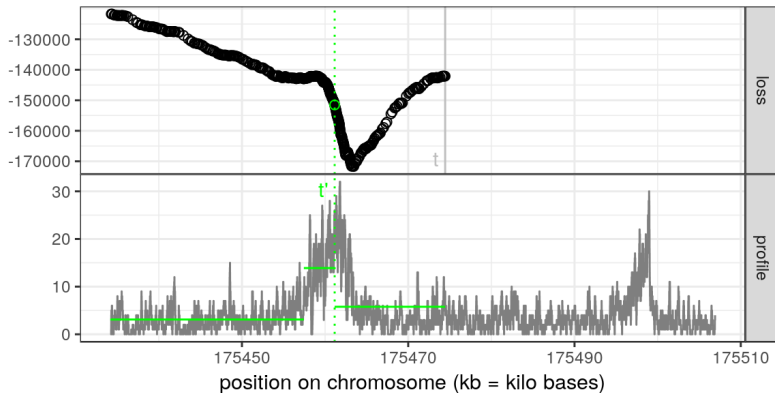
\vdots

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



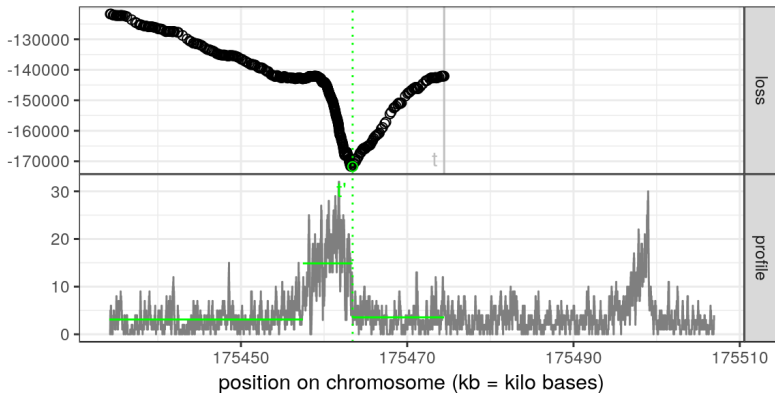
$$\mathcal{L}_{3,t} = \min_{t' < t} \underbrace{\mathcal{L}_{2,t'}}_{\text{optimal loss in 2 segments up to } t'} + \underbrace{C_{(t',t]}}_{\text{optimal loss of 3rd segment } (t', t]}$$

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



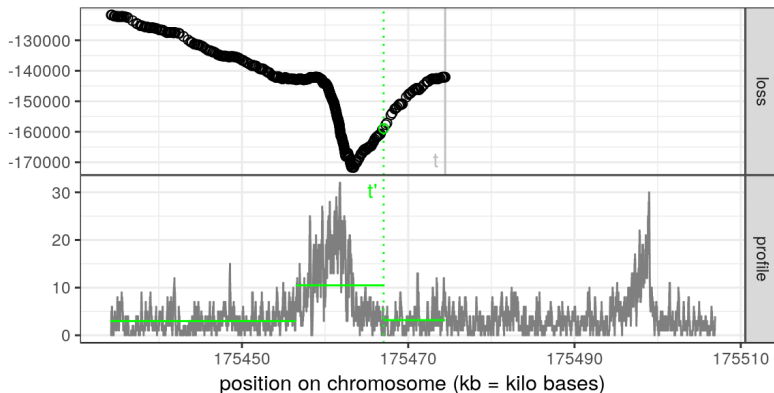
$$\mathcal{L}_{3,t} = \min_{t' < t} \underbrace{\mathcal{L}_{2,t'}}_{\text{optimal loss in 2 segments up to } t'} + \underbrace{C_{(t',t]}}_{\text{optimal loss of 3rd segment } (t', t]}$$

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



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

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



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

Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

Theoretical time complexity

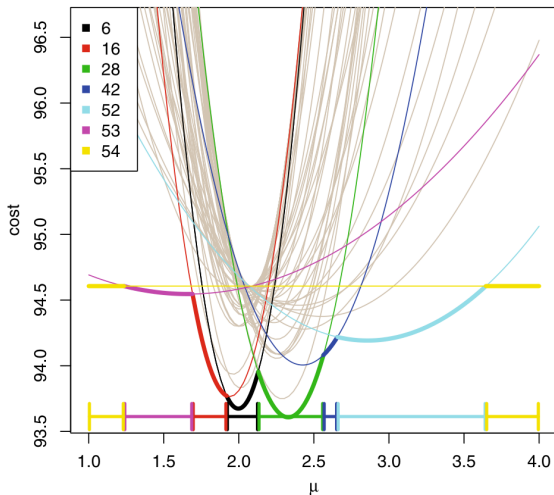
Classical dynamic programming is too slow for big data

- ▶ 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 :

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

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

Theoretical time complexity

Number of intervals in real and simulated data

Rigaill, arXiv:1004.0887.

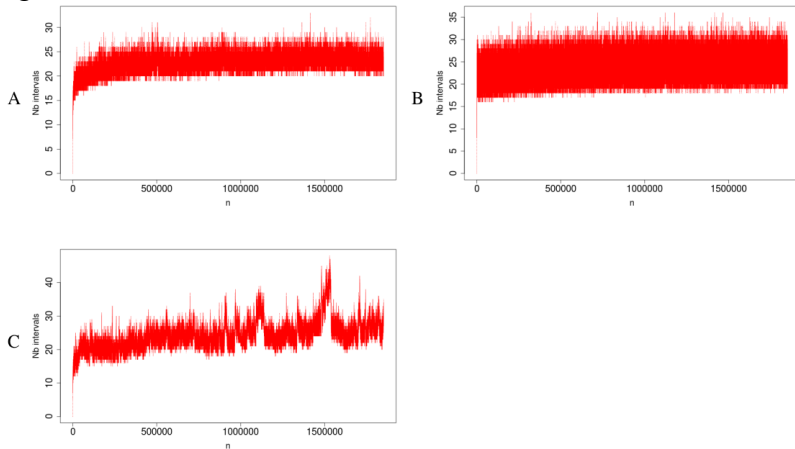
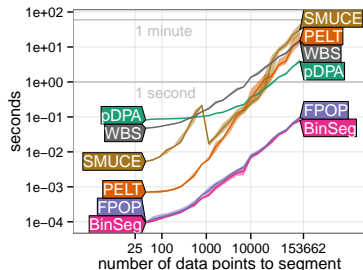
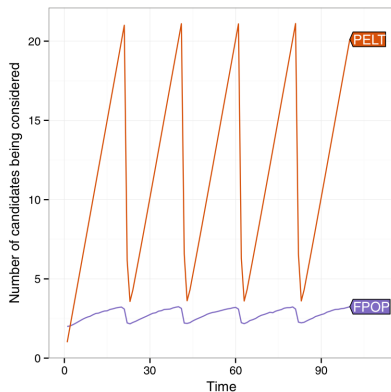


FIGURE 5. Maximum number of intervals stored by the pDPA at each point of the sequence for $K = 1$. A: For 100 sequences of $1.8 \cdot 10^6$ points simulated with a constant signal plus an additional normal noise of variance 1. B: For 100 sequences of $1.8 \cdot 10^6$ points simulated with a sine wave 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.* Journal of Machine Learning Research 21(87):1–40, 2020.

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

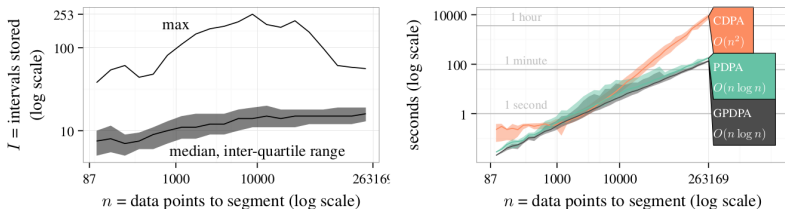
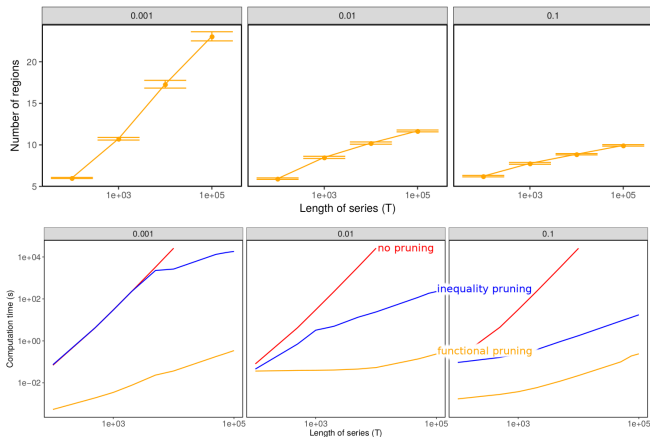


Figure 3: Empirical speed analysis on 2752 count data vectors from the histone mark ChIP-seq benchmark. For each vector we ran the GPDPA with the up-down constraint and a max of $K = 19$ segments. The expected time complexity is $O(KnI)$ where I is the average number of intervals (function pieces; candidate 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.

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

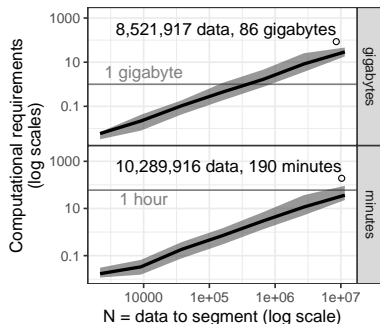
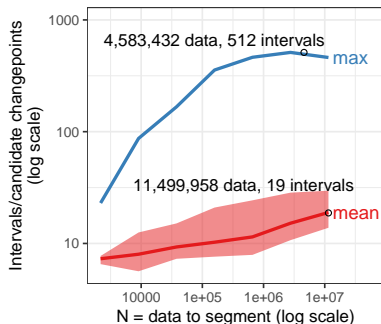


Another fast constrained algorithm for genomics

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

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

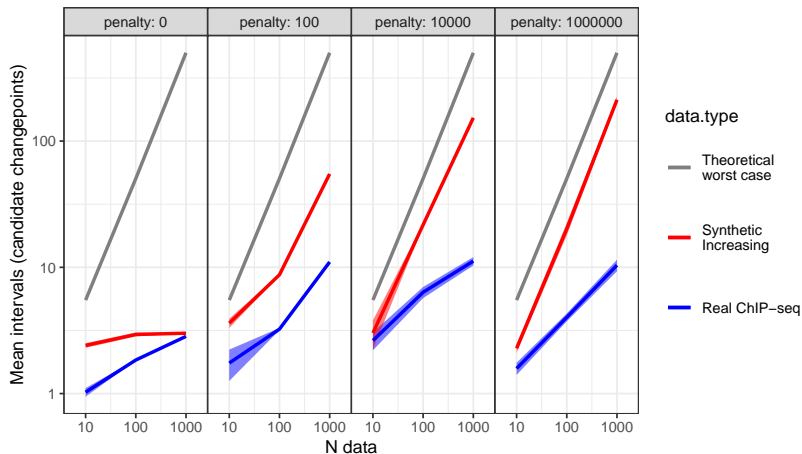
subject to ...up-down constraints on m .



$I = O(\log n)$ 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.

Classical dynamic programming for optimal changepoint detection

Functional pruning algorithms

Empirical time complexity

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

Dynamic programming recursion with functional pruning

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

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

Example data set with $n = 4$

Rigaill, arXiv:1004.0887.

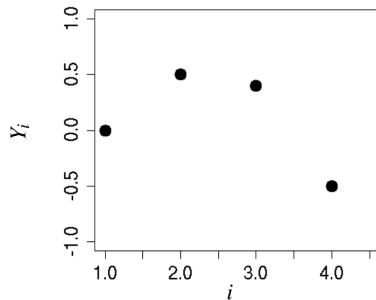
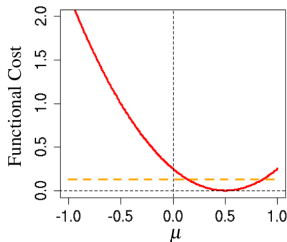


FIGURE 1. *Four-point signal. y_i as a function of i . $y_1 = 0$, $y_2 = 0.5$, $y_3 = 0.4$, $y_4 = -0.5$*

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 $\tau = 3$: $\mathcal{L}_{1,2}$.



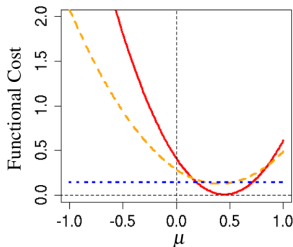
τ	Functional cost	$\mathcal{S}_{1:3,\tau}^1$
2	$0.25 - \mu + \mu^2$	$[0.146, 0.854]$
3	0.125	$[-\infty, 0.146] \cup [0.854, +\infty]$

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 $\tau = 4$:
 $\mathcal{L}_{1,3} = \min_{\mu}(\mu - 0)^2 + (\mu - 0.5)^2 + (\mu - 0.4)^2$.

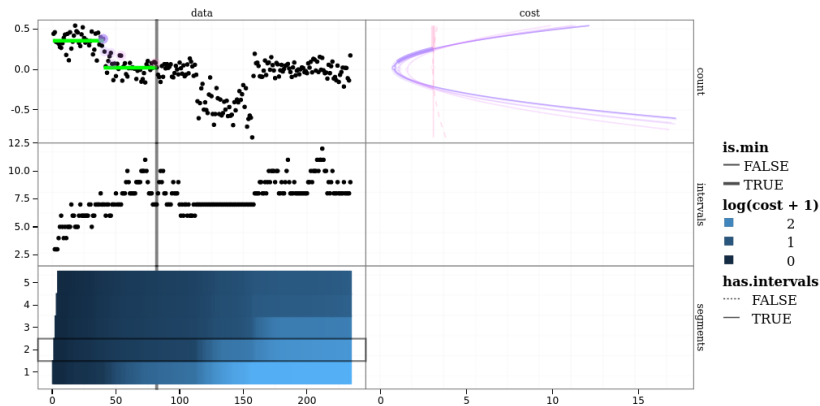


τ	Functional cost	$\mathcal{S}_{1:4,\tau}^1$
2	$0.41 - 1.8\mu + 2\mu^2$	$[0.190, 0.709]$
3	$0.285 - 0.8\mu + \mu^2$	\emptyset
4	0.14	$[-\infty, 0.190] \cup [0.709, +\infty]$

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/>