

# Detecting changes in slope with an $L_0$ penalty

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## Abstract

Whilst there are many approaches to detecting changes in mean for a univariate time-series, the problem of detecting multiple changes in slope has comparatively been ignored. Part of the reason for this is that detecting changes in slope is much more challenging. For example, simple binary segmentation procedures do not work for this problem, whilst efficient dynamic programming methods that work well for the change in mean problem cannot be directly used for detecting changes in slope. We present a novel dynamic programming approach, CPOP, for finding the “best” continuous piecewise-linear fit to data. We define best based on a criterion that measures fit to data using the residual sum of squares, but penalises complexity based on an  $L_0$  penalty on changes in slope. We show that using such a criterion is more reliable at estimating changepoint locations than approaches that penalise complexity using an  $L_1$  penalty. Empirically CPOP has good computational properties, and can analyse a time-series with over 10,000 observations and over 100 changes in a few minutes. Our method is used to analyse data on the motion of bacteria, and provides fits to the data that both have substantially smaller residual sum of squares and are more parsimonious than two competing approaches.

**Keywords:** Breakpoints, Changepoint, Functional Pruning, Linear Spline Regression, Narrowest-over-threshold, Optimal partitioning, Trend-filtering

## 1 Introduction

Changepoint detection and modelling is currently one of the most active research areas in statistics due to its importance across a wide range of applications, including: finance (Fryzlewicz, 2014);

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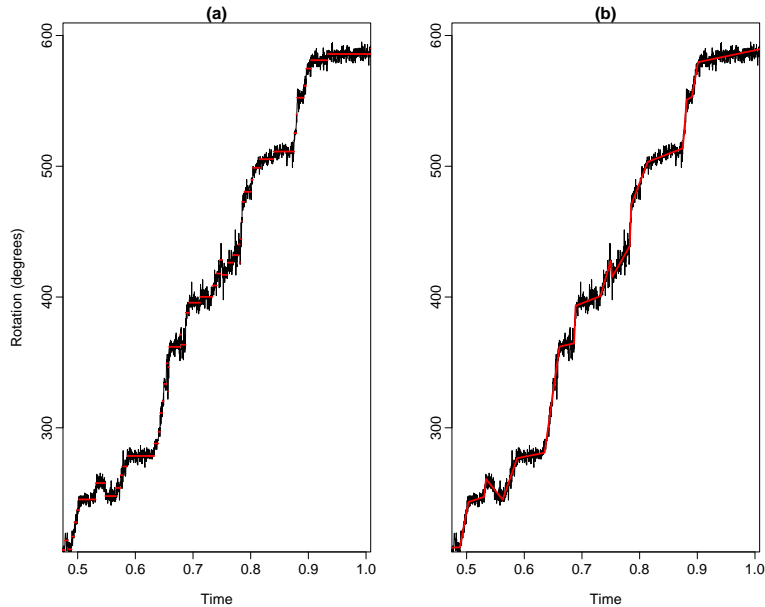


Figure 1: Part of a time-series of angular position of a bacterium, taken from Sowa et al. (2005); best fitting piecewise constant mean (a) and continuous piecewise-linear mean (b).

bioinformatics (Futschik et al., 2014; Hocking et al., 2014); environmental science (Killick et al., 2010); target tracking (Nemeth et al., 2014); fMRI (Aston and Kirch, 2012); and biochemistry (Hotz et al., 2013) amongst many others. It appears to be increasingly important for the analysis of large scale data streams, as it is a flexible way of modelling non-stationarity or heterogeneity in these streams. Change-point detection has been identified as one of the major challenges for modern, big data applications (National Research Council, 2013). This paper focusses on the problem of detecting changes in slope. That is, we consider data whose mean varies over time, and where we model this mean as a continuous piecewise-linear function of time.

To motivate this work consider the challenge of analysing data of the angular position and velocity of a bacterium, see Figure 1. The interest is in understanding the movement of the bacterium. The movement is driven by the bacterial flagella, a slender thread-like structure that enables the bacteria to swim. The movement is circular, and thus the position of a bacterium at any time point can be summarised by its angular position. The data we show comes from Sowa et al. (2005) and was obtained by first taking images of the bacterium at high-frequency. From these images the angular position is calculated at each time-point. The motion is then summarised by a time-series of the amount of rotation that the bacterium has done from its initial position.

The interest from such data is in deriving understanding about the bacterial flagella motor. In particular the angular motion is characterised by stationary periods interspersed by periods of roughly constant angular velocity. The movement tends to be, though is not exclusively, in one direction.

Weinmann and Storath (2015) analyse this data using a changepoint model, where the mean is piecewise constant. An example fit from such a model is shown in 1(a). This model is not a natural model given the underlying physics of the application, and this can be seen in how it tries to fit periods of rotation by a number of short stationary regimes. A more natural model is one whereby we segment the data into periods of constant angular velocity. Such a model is equivalent to fitting a continuous piecewise-linear mean function to the data, with the slope of this function in each segment corresponding to the angular velocity in the segment. Such a fit is shown in 1(b).

Whilst detecting changes in slope seems to be a similar statistical problem to detecting changes in mean, it is fundamentally more challenging. For example, binary segmentation approaches (Scott and Knott, 1974; Fryzlewicz, 2014), which are the most popular generic approach to detecting multiple changepoints, do not work for detecting changes in slope (as shown by Baranowski et al., 2016). Binary segmentation iteratively applies a method for detecting a single changepoint. For change in slope problems one can show that for some underlying signals, initial estimates of changepoint locations will tend to be midway between actual changepoint locations; binary segmentation is unable to then recover from such incorrect initial estimates.

The standard approach to detecting changes in mean is to attempt to find the “best” piecewise-constant mean function, where best is defined based on its fit to the data penalised by a measure of complexity of the mean function (Yao, 1988; Lavielle and Moulines, 2000). The most common measure of fit is through the residual sum of squares, and the most natural measure of complexity is the number of changepoints. The latter corresponds to an  $L_0$  penalty on the change in the slope of the mean. Dynamic programming can be used to efficiently find the best segmentation of the data under such a criterion for the change in mean problem (Jackson et al., 2005; Killick et al., 2012; Maidstone et al., 2017).

Our statistical approach is to use the same framework to detect changes in slope. We aim to find the best continuous piecewise-linear mean function, where best is defined in terms of the residual sum of squares plus a penalty that depends on the number of changepoints. However standard dynamic programming algorithms cannot be directly applied to such a problem. The assumption of continuity introduces dependencies in the parameters associated with each segment, and these in turn violate the conditional independence structure that existing dynamic programming algorithms use. In fact Weinmann and Storath (2015) report that detecting changes in slope under this criterion lies within a class of NP-hard problems and claim that “for real applications, there is no hope to find a global minimizer in reasonable time”. Despite this claim, we present a dynamic programming algorithm that does find the best segmentation under this criterion, and has practicable computational cost – of the order of minutes when analysing 10,000 data points with of the order of 100 changepoints.

There has been earlier work on detecting changes in slope using the same or similar statistical criteria. These include Tomé and Miranda (2004) who use an exhaustive search to find the best segmentation – an approach that is only feasible for very small data sets, with perhaps at most 100 to 200 data points. Alternatively, approximate solutions to the true optimal segmentation are found, for example by discretising the locations in time and space where changes can occur (Goldberg et al., 2014) or by using a genetic algorithm to approximately solve the optimisation problem (Horner and Beauchamp, 1996). As we show, our novel dynamic programming approach is guaranteed to find the best segmentation under our criterion, and is still computationally feasible for large data sets. Empirical results suggest the expected computational cost of our algorithm is slightly worse than quadratic in the number of data points, and can be close to linear in situations where the number of changepoints increases linearly with the number of data points.

The outline of the paper is as follows. The next section defines the statistical criterion that we use for detecting changes in slope, and defines the optimisation problem we wish to solve in order to find the best segmentation of the data. We present our dynamic programming algorithm, which we call CPOP, in Section 3. We then empirically evaluate the computational and statistical performance of CPOP. For the latter we compare with trend-filtering (Tibshirani, 2014) and the narrowest-over-threshold (NOT) approach (Baranowski et al., 2016). The former involves replacing the  $L_0$  penalty on changes in slope with an  $L_1$  penalty, so that we penalise mean functions based on how much, rather than the number of times, their slope changes. This makes the resulting optimisation problem convex, and hence easy to solve. However we show that whilst trend-filtering can estimate the underlying mean function well, it never performs well at accurately detecting where the changes occur. The NOT approach is a novel version of binary segmentation that can be shown to give consistent estimation of changepoint locations for our change in slope model. Our results show it performs well at detecting and estimating the location of the changepoints, but is less accurate than CPOP at estimating the underlying mean. In Section 5 we analyse the data from Figure 1. We give statistical evidence that a change in slope model is better than fitting either a piecewise-constant or a discontinuous piecewise-linear mean function to the data. We also show that CPOP is able to find much better fitting estimates of the mean with substantially fewer changepoints than either trend-filtering or NOT. Finally, the dynamic programming approach we present in this paper can be applied to a larger range of changepoint problems than the change in slope problem we consider. These possible extensions are discussed in Section 6.

## 2 Model Definition

We assume that we have data ordered by time and denote this by  $\mathbf{y} = (y_1, \dots, y_n)$ . We will also use the notation that for  $t \geq s$  the set of observations from time  $s$  to time  $t$  is  $\mathbf{y}_{s:t} = (y_s, \dots, y_t)$ . If we assume that there are  $m$  changepoints in the data, this will correspond to the data being split into  $m + 1$  distinct segments. We let the location of the  $j$ th changepoint be  $\tau_j$  for  $j = 1, \dots, m$ , and set  $\tau_0 = 0$  and  $\tau_{m+1} = n$ . The  $j$ th segment will consist of data points  $y_{\tau_{j-1}+1}, \dots, y_{\tau_j}$ . We let  $\boldsymbol{\tau} = (\tau_0, \dots, \tau_{m+1})$  be the set of ordered changepoints.

We consider the case of fitting a continuous piecewise linear function to the data. An example of such a fit is given in the right-hand plot of Figure 1. For such a problem, changepoints will correspond to points in time where the slope of the function changes. There are a variety of ways of parameterising the linear function within each segment. Due to the continuity constraint that we wish to enforce it is helpful to parameterise this linear function by its value at the start and its value at the end of the segment. Our continuity constraint then requires this value for the end of one segment to be equal to the value at the start of the next segment. For the changepoint  $\tau_i$  we will denote this common value as  $\phi_{\tau_i}$ . A continuous piecewise linear function is then defined by the set of changepoints, and these values of the linear function at the changes,  $\phi_{\tau_i}$  for  $i = 0, \dots, m + 1$ . As for the changepoints, we will simplify notation slightly by letting  $\boldsymbol{\phi} = (\phi_{\tau_0}, \dots, \phi_{\tau_{m+1}})$ . In situations where we refer to a subset of this vector we will use the notation  $\boldsymbol{\phi}_{j:k} = (\phi_{\tau_j}, \dots, \phi_{\tau_k})$  for  $0 \leq j \leq k \leq m + 1$ .

Under this parameterisation, we model the data as, for  $i = 0, \dots, m$ ,

$$Y_t = \phi_{\tau_i} + \frac{\phi_{\tau_{i+1}} - \phi_{\tau_i}}{\tau_{i+1} - \tau_i} (t - \tau_i) + Z_t, \quad \text{for } t = \tau_i + 1, \dots, \tau_{i+1}, \quad (1)$$

where  $Z_t$ , for  $t = 1, \dots, n$ , are independent, zero-mean, random variables with common variance  $\sigma^2$ .

Our aim is to infer the set of changepoints, and the underlying piecewise linear function, from the data. Our approach to doing this is based on a penalised cost approach, using a squared-error loss function to measure fit to the data. That is, we wish to minimise over  $m$ ,  $\boldsymbol{\tau}$ , and  $\boldsymbol{\phi}$ ,

$$\sum_{i=0}^m \left[ \frac{1}{\sigma^2} \sum_{t=\tau_i+1}^{\tau_{i+1}} \left( y_t - \phi_{\tau_i} - \frac{\phi_{\tau_{i+1}} - \phi_{\tau_i}}{\tau_{i+1} - \tau_i} (t - \tau_i) \right)^2 + h(\tau_{i+1} - \tau_i) \right] + \beta m, \quad (2)$$

for some suitable choice of penalty constant  $\beta > 0$  and segment-length penalty function  $h(\cdot)$ . These penalties are needed to avoid over-fitting of the data. Perhaps the most common choice of penalty is BIC (Schwarz, 1978), where  $\beta = 2 \log(n)$  and  $h(s) = 0$  for all segment lengths  $s$ . However, it has been shown that allowing the penalty to depend on segment length can improve the accuracy of penalised cost approaches, and such penalties have been suggested through a modified BIC penalty

(Zhang and Siegmund, 2007) and within the minimum description length approach (Davis et al., 2006). The above cost function assumes knowledge of the noise variance,  $\sigma^2$ . In practice this is not known and needs to be estimated, for example using the Median Absolute Deviation estimator (Hampel, 1974); see for example Fryzlewicz (2014).

We can simplify (2) through introducing segment costs. Define the segment cost for fitting the mean of the data  $\mathbf{y}_{s+1:t}$  with a linear function that starts at  $\phi$  at time  $s$  and ends at  $\psi$  at time  $t$  as

$$\mathcal{C}(\mathbf{y}_{s+1:t}, \phi, \psi) = \frac{1}{\sigma^2} \sum_{j=s+1}^t \left( y_j - \phi - \frac{\psi - \phi}{t - s} (j - s) \right)^2. \quad (3)$$

Then we wish to estimate the number and location of the changepoints, and the underlying continuous piecewise-linear function through solving the following minimisation problem:

$$\min_{\tau, m, \phi} \left\{ \sum_{i=0}^m [\mathcal{C}(\mathbf{y}_{\tau_i+1:\tau_{i+1}}, \phi_{\tau_i}, \phi_{\tau_{i+1}}) + h(\tau_{i+1} - \tau_i)] + \beta(m + 1) \right\}. \quad (4)$$

### 3 Minimising the Penalised Cost

Solving the minimisation problem in (4) by complete enumeration takes  $\mathcal{O}(2^n)$  time and therefore is infeasible for large values of  $n$ . Below we propose a pruned dynamic programming approach to calculate the exact solution to (4) efficiently. This dynamic programming approach is much more complicated than other dynamic programming algorithms used in changepoint detection as neighbouring segments share a common parameter: the end-point of the piecewise linear function for one segment is the start-point of this function for the next segment.

Dynamic programming requires a conditional separability property. We need to be able to choose some information at time  $s$  such that, conditional on this information, we can separately minimise the cost related to the data before and after  $s$ . For simpler changepoint problems, this information is just the presence of a changepoint at  $s$ : as conditional on this, we can separately find the best segmentation of the data before  $s$  and the best segmentation of the data after  $s$ . For our changepoint problem, the fact that neighbouring segments share a parameter means that conditioning just on the presence of a changepoint at  $s$  will no longer give us the required separability. Instead, we will introduce a continuous-state dynamic programming algorithm which conditions on both the location of a changepoint at  $s$  and the value of the function at  $s$ . The idea is that given both these pieces of information we can separately find the best segmentation of the data before  $s$  and the best segmentation of the data after  $s$ .

### 3.1 Dynamic Programming Approach

Consider segmenting the data up to time  $t$ ,  $\mathbf{y}_{1:t}$ , for  $t = 1, \dots, n$ . When segmenting  $\mathbf{y}_{1:t}$  with  $k$  changepoints,  $\tau_1, \dots, \tau_k$ , we use the notation  $\tau_0 = 0$  and  $\tau_{k+1} = t$ . We define the function  $f^t(\phi)$  to be the minimum penalised cost for segmenting  $\mathbf{y}_{1:t}$  conditional on  $\phi_t = \phi$ , that is the fitted value at time  $t$  is  $\phi$ . Formally this is defined as

$$f^t(\phi) = \min_{\boldsymbol{\tau}, k, \phi_{0:k}} \left\{ \sum_{i=0}^{k-1} [\mathcal{C}(\mathbf{y}_{\tau_i+1:\tau_{i+1}}, \phi_{\tau_i}, \phi_{\tau_{i+1}}) + h(\tau_{i+1} - \tau_i)] + [\mathcal{C}(\mathbf{y}_{\tau_k+1:t}, \phi_{\tau_k}, \phi) + h(t - \tau_k)] + \beta(k+1) \right\}. \quad (5)$$

By manipulating (5), and using the initial condition that  $f^0(\phi) = 0$ , we can construct a dynamic programming recursion for  $f^t(\phi)$ .

$$\begin{aligned} f^t(\phi) &= \min_{\boldsymbol{\tau}, k, \phi_{0:k}} \left\{ \sum_{i=0}^{k-1} [\mathcal{C}(\mathbf{y}_{\tau_i+1:\tau_{i+1}}, \phi_{\tau_i}, \phi_{\tau_{i+1}}) + h(\tau_{i+1} - \tau_i)] + \beta k \right. \\ &\quad \left. + \mathcal{C}(\mathbf{y}_{\tau_k+1:t}, \phi_{\tau_k}, \phi) + h(t - \tau_k) + \beta \right\}, \\ &= \min_{\phi', s} \left\{ \min_{\boldsymbol{\tau}_{0:k-1}, k, \phi_{0:k-1}} \left\{ \sum_{i=0}^{k-2} [\mathcal{C}(\mathbf{y}_{\tau_i+1:\tau_{i+1}}, \phi_{\tau_i}, \phi_{\tau_{i+1}}) + h(\tau_{i+1} - \tau_i)] + \right. \right. \\ &\quad \left. \left. + \mathcal{C}(\mathbf{y}_{\tau_{k-1}+1:s}, \phi_{\tau_{k-1}}, \phi') + h(s - \tau_{k-1}) + \beta k \right\} + \mathcal{C}(\mathbf{y}_{s+1:t}, \phi', \phi) + h(t - s) + \beta \right\}, \\ &= \min_{\phi', s} \{ f^s(\phi') + \mathcal{C}(\mathbf{y}_{s+1:t}, \phi', \phi) + h(t - s) + \beta \}. \end{aligned}$$

The idea is that we split the minimisation into first minimising over the time of the most recent changepoint and the fitted value at that changepoint, and then minimising over the earlier changepoints and fitted values. On the third line we let  $s$  denote the time of the most recent changepoint, and  $\phi'$  the fitted value at  $s$ . The inner minimisation is over the number of changepoints, the locations of those changepoints prior to  $s$ , and the fitted values at the changepoints prior to  $s$ . This inner minimisation gives the minimum penalised cost for segmenting  $\mathbf{y}_{1:s}$  conditional on  $\phi_s = \phi'$ , which is  $f^s(\phi')$ . This recursion is similar to that derived for Optimal Partitioning. However for Optimal Partitioning we just needed to store a scalar value for each  $t = 1, \dots, n$ . Here we need to store functions of the continuous parameter  $\phi$  for each value of  $t$ .

To store  $f^t(\phi)$  we will write it as the point-wise minimum of a set of cost functions of  $\phi$ , each of which corresponds to a different vector of changepoints,  $\boldsymbol{\tau}$ . We define each of these functions  $f_{\boldsymbol{\tau}}^t(\phi)$  as the minimum cost of segmenting  $\mathbf{y}_{1:t}$  with changepoints at  $\boldsymbol{\tau} = \tau_1, \dots, \tau_k$  and fitted value at time

$t$  being  $\phi$ :

$$f_{\boldsymbol{\tau}}^t(\phi) = \min_{\phi_{0:k}} \left\{ \sum_{i=0}^{k-1} [\mathcal{C}(\mathbf{y}_{\tau_i+1:\tau_{i+1}}, \phi_{\tau_i}, \phi_{\tau_{i+1}}) + h(\tau_{i+1} - \tau_i)] \right. \\ \left. + \mathcal{C}(\mathbf{y}_{\tau_k+1:t}, \phi_{\tau_k}, \phi) + h(t - \tau_k) + \beta(k + 1) \right\}. \quad (6)$$

Then  $f^t(\phi)$  is the point-wise minimum of these functions,

$$f^t(\phi) = \min_{\boldsymbol{\tau} \in \mathcal{T}_t} f_{\boldsymbol{\tau}}^t(\phi), \quad (7)$$

where we define  $\mathcal{T}_t$  to be the set of all possible changepoint vectors at time  $t$ .

Each of the above functions,  $f_{\boldsymbol{\tau}}^t(\phi)$ , is a quadratic in  $\phi$  and thus can be represented by a vector of length 3, with the terms in this vector denoting the co-efficients of the quadratic. We can calculate the co-efficients recursively using

$$f_{\boldsymbol{\tau}}^t(\phi) = \min_{\phi'} \left\{ f_{\tau_1, \dots, \tau_{k-1}}^{\tau_k}(\phi') + \mathcal{C}(\mathbf{y}_{\tau_k+1:t}, \phi', \phi) + h(t - \tau_k) + \beta \right\}. \quad (8)$$

Further details are given in Appendix A. Therefore we can iteratively compute these functions and thus calculate  $f^n(\phi)$ .

We then calculate the optimal segmentation of  $\mathbf{y}_{1:n}$  by minimising  $f^n(\phi)$  over  $\phi$ . The value of  $\boldsymbol{\tau}$  that achieves the minimum value will be the optimal segmentation. This approach, however, is computationally expensive; both in time,  $\mathcal{O}(n2^n)$ , and space needed to store the functions,  $\mathcal{O}(2^n)$ . To obtain a practicable algorithm we have to use pruning ideas to reduce the number of changepoint vectors, and corresponding functions  $f_{\boldsymbol{\tau}}^t(\phi)$ , that we need to store. There are two ways in which this can be achieved: functional pruning and inequality based pruning. In both cases they are able to remove changepoint vectors whilst still maintaining the guarantee that the resulting algorithm will find the true minimum of the optimisation problem (2).

## 3.2 Functional Pruning

One way we can prune these candidate changepoint vectors from the minimisation problem is when they can be shown to be dominated by other vectors for any given value of  $\phi$ . Similar approaches are found in Rigaiil (2015) and Maidstone et al. (2017) for independent segment models and is known as *functional pruning*.

In Theorem 3.1 we show how if a candidate changepoint vector,  $\boldsymbol{\tau}$  is not optimal at time  $s$  for any value of  $\phi$ , then the related candidate changepoint vector  $(\boldsymbol{\tau}, s)$  (the concatenation of  $\boldsymbol{\tau}$  and  $s$ ) is not optimal for any value of  $\phi$  at time  $t$  where  $t > s$ . If this is the case, the vector  $(\boldsymbol{\tau}, s)$  can be pruned from the candidate changepoint set.



First we define the set  $\mathcal{T}_t^*$  as the set of changepoint vectors that are optimal for some  $\phi$  at time  $t$

$$\mathcal{T}_t^* = \{\boldsymbol{\tau} \in \mathcal{T}_t : f^t(\phi) = f_{\boldsymbol{\tau}}^t(\phi), \text{ for some } \phi \in (-\infty, \infty)\}, \quad (9)$$

where  $\mathcal{T}_t$  is the set of all possible changepoint vectors at time  $t$ . If a candidate vector  $\boldsymbol{\tau}$  is not in this set at time  $s$  then the related candidate vector  $(\boldsymbol{\tau}, s)$  is not in the set at time  $t$ . This means that at time  $t$  we will need to store only the functions  $f_{\boldsymbol{\tau}}^t(\phi)$  corresponding to segmentations that are in  $\mathcal{T}_t^*$ .

**Theorem 3.1** *If  $\boldsymbol{\tau} \notin \mathcal{T}_s^*$  then  $(\boldsymbol{\tau}, s) \notin \mathcal{T}_t^*$  for all  $t > s$ .*

**Proof:** See Appendix B.

The key to an efficient algorithm will be a way of efficiently calculating  $\mathcal{T}_t^*$ . We can use the above theorem to help us do this. From Theorem 3.1 we can define a set

$$\hat{\mathcal{T}}_t = \left\{ (\boldsymbol{\tau}, s) : s \in \{0, \dots, t-1\}, \boldsymbol{\tau} \in \mathcal{T}_s^* \right\}, \quad (10)$$

and we will have that  $\hat{\mathcal{T}}_t \supseteq \mathcal{T}_t^*$ . So assume that we have calculated the sets  $\mathcal{T}_s^*$  for  $s = 0, \dots, t-1$ . We can calculate  $f_{\boldsymbol{\tau}}^t(\phi)$  only for  $\boldsymbol{\tau} \in \hat{\mathcal{T}}_t$ . When calculating  $f^t(\phi)$ , as defined by (7), we can just minimise over the set of changepoint vectors in  $\hat{\mathcal{T}}_t$  rather than the full set. Furthermore we can calculate which of the sets of changepoints in  $\hat{\mathcal{T}}_t$  contribute to this minimum and remove those that do not contribute. The remaining sets of changepoints define  $\mathcal{T}_t^*$ .

To find out which sets of changepoints,  $\boldsymbol{\tau}$ , contribute to the minimisation of (7) we store the interval (or set of intervals) of  $\phi$  space for which it is optimal. We define this interval as follows

$$Int_{\boldsymbol{\tau}}^t = \left\{ \phi : f_{\boldsymbol{\tau}}^t(\phi) = \min_{\boldsymbol{\tau}' \in \hat{\mathcal{T}}_t} f_{\boldsymbol{\tau}'}^t(\phi) \right\}. \quad (11)$$

For a given  $t$  the union of these intervals over  $\boldsymbol{\tau}$  is just the real line (as for a given  $\phi$  at least one changepoint vector  $\boldsymbol{\tau}$  corresponds to the optimal segmentation). Using this we can derive a simple algorithm for updating these intervals which involves a search over the real line, recursively finding the function, and associated interval, which is optimal as we increase  $\phi$  from  $-\infty$  to  $\infty$ . This method is given in full in Algorithm 2, and there is a detailed explanation in Appendix C.

Having calculated  $Int_{\boldsymbol{\tau}}^t$  for all  $\boldsymbol{\tau} \in \hat{\mathcal{T}}_t$  we can use these to calculate  $\mathcal{T}_t^*$ . We remove  $\boldsymbol{\tau}$  from  $\hat{\mathcal{T}}_t$  if  $Int_{\boldsymbol{\tau}}^t = \emptyset$  and after doing this for all  $\boldsymbol{\tau} \in \hat{\mathcal{T}}_t$  we are left with precisely those values of  $\boldsymbol{\tau}$  which make up  $\mathcal{T}_t^*$ . This is used to recursively calculate  $\hat{\mathcal{T}}_{t+1}$

$$\hat{\mathcal{T}}_{t+1} = \hat{\mathcal{T}}_t \cup \left\{ (\boldsymbol{\tau}, t) : \boldsymbol{\tau} \in \mathcal{T}_t^* \right\}. \quad (12)$$

### 3.3 Inequality Based Pruning

A further way pruning can be used to speed up the dynamic programming algorithm is by applying *inequality based pruning* (Maidstone et al., 2017), a similar idea to the pruning step used in the PELT algorithm (Killick et al., 2012). This pruning is based on the following result.

**Theorem 3.2** *Define  $K = 2\beta + h(1) + h(n)$ . If  $h(\cdot)$  is a non-negative, non-decreasing function and if for some  $\tau$ ,*

$$\min_{\phi} f_{\tau}^t(\phi) > \min_{\phi'} [f^t(\phi')] + K, \quad (13)$$

*then at any future time  $T$ , the set of changepoints  $\tau$  can never be optimal for the data  $\mathbf{y}_{1:T}$ .*

**Proof:** See Appendix B.

This result states that for any candidate changepoint vector, if the best cost at time  $t$  is worse than the best cost over all changepoint vectors plus  $K$ , we can show that the candidate is sub-optimal at all future times as well. In Section 3.2 we considered candidate changepoints vectors that belonged to the set  $\hat{\mathcal{T}}_t$ , and updated the related cost functions. We then used functional pruning to reduce this set to only those values that are optimal for some value of  $\phi$ , namely the set  $\mathcal{T}^*$ . Using Theorem 3.2 we can reduce the size of  $\hat{\mathcal{T}}_{t+1}$  before the cost functions are updated, discarding candidates from the set if (13) is true. As this reduces the size of the set  $\hat{\mathcal{T}}_t$ , it also reduces the computational cost of the algorithm.

Both pruning steps can be used to restrict the set of candidate changepoint vectors that the dynamic program is run over. We call the resulting algorithm CPOP, for Continuous-piecewise-linear Pruned Optimal Partitioning. The pseudocode for the full method with these pruning steps is outlined in Algorithm 1 in the Appendix.

### 3.4 Computational Cost of CPOP

The computational cost of the CPOP algorithm depends crucially on the size of  $\mathcal{T}_t^*$  and  $\hat{\mathcal{T}}_t$ . Denote the size of each set by  $|\mathcal{T}_t^*|$  and  $|\hat{\mathcal{T}}_t|$  respectively. For iteration  $t$  of the CPOP, the cost of calculating the quadratics,  $f_{\tau}^t(\phi)$ , associated with each  $\tau \in \hat{\mathcal{T}}_t$ , will be linear in  $|\hat{\mathcal{T}}_t|$ . The cost of calculating  $Int_{\tau}^t$ , the intervals of  $\phi$  for which each quadratic is optimal, will have a cost that is of the order of  $|\hat{\mathcal{T}}_t|$  times the number of disjoint intervals that contribute to the set of  $Int_{\tau}^t$ . We believe the number of such intervals increases linearly in  $|\mathcal{T}_t^*|$ . Note that without the inequality-based pruning we have  $|\hat{\mathcal{T}}_t| = \sum_{s=1}^{t-1} |\mathcal{T}_s^*|$ .

To investigate empirically how the size of these sets increase with  $t$ , and what the resulting computational cost of CPOP is, we analysed simulated data sets of different sizes,  $n$ , and with differ-

ent numbers of changepoints,  $m$ . For a given choice of  $n$  and  $m$  we set the changepoints to be equally spaced, and simulated the value of the underlying mean function at the each changepoint as an independent draw from a Gaussian distribution with variance 4. We then simulated data by adding independent, identically distributed standard Gaussian noise to this mean function at each time-point. We present results for  $n = 1000$  and for both many changepoints,  $m = 19$ , and no changepoint,  $m = 0$  in Figure 2 (qualitatively similar results were obtained for other values of  $n$  and  $m$ ).

Without pruning, the value of  $|\mathcal{T}_t^*|$  would increase exponentially with  $t$ . However we see that in both cases  $|\mathcal{T}_t^*|$  remains small for all  $t$ , with the average values always less than 20.

The behaviour of  $|\mathcal{T}_t^*|$  is different for the two cases. For the no changepoint case, the size of this set increases linearly with  $t$ . For the many changepoint case the size initially increases linearly but then appears roughly constant. The reason for this is that the inequality based pruning of Section 3.3 is able to prune many of the segmentations in  $|\mathcal{T}_t^*|$  that have a most recent changepoint which is a long-time prior to the actual most recent changepoint (see Killick et al., 2012, for a similar effect of this type of pruning). This reduces the size of  $|\mathcal{T}_t^*|$  substantially when there are many changepoints, whereas the inequality based pruning has almost no effect for the case where there are no changepoints.

We also empirically investigated the overall computational cost of CPOP for different sizes of data set,  $n$ , and different numbers of changepoints,  $m$ . Figure 3 shows the average time for CPOP. The first plot is of computational cost against  $n$  for three different regimes for  $m$ . For each of the three regimes we see a roughly linear relationship between the log computational cost and  $\log(n)$ . The slopes of these lines vary between 1.3 for the fixed  $m$  regime and 2.3 for the regime where  $m$  increases linearly with  $n$ . These suggest computational cost grows like  $n^{1.3}$  and  $n^{2.3}$  respectively. This is consistent with the second plot, which shows that for fixed  $n$  the computational cost decreases with increasing  $m$ .

## 4 Statistical Performance of CPOP

We now look empirically at the statistical performance of CPOP, and compare this with two other methods for fitting a continuous piecewise-linear mean function to data and detecting the locations where the slope of this function changes.

The most common, general, approach for detecting changes is to use binary segmentation (Scott and Knott, 1974), but as mentioned in the introduction binary segmentation does not work for this problem: there are examples where even if you observed the underlying mean function without

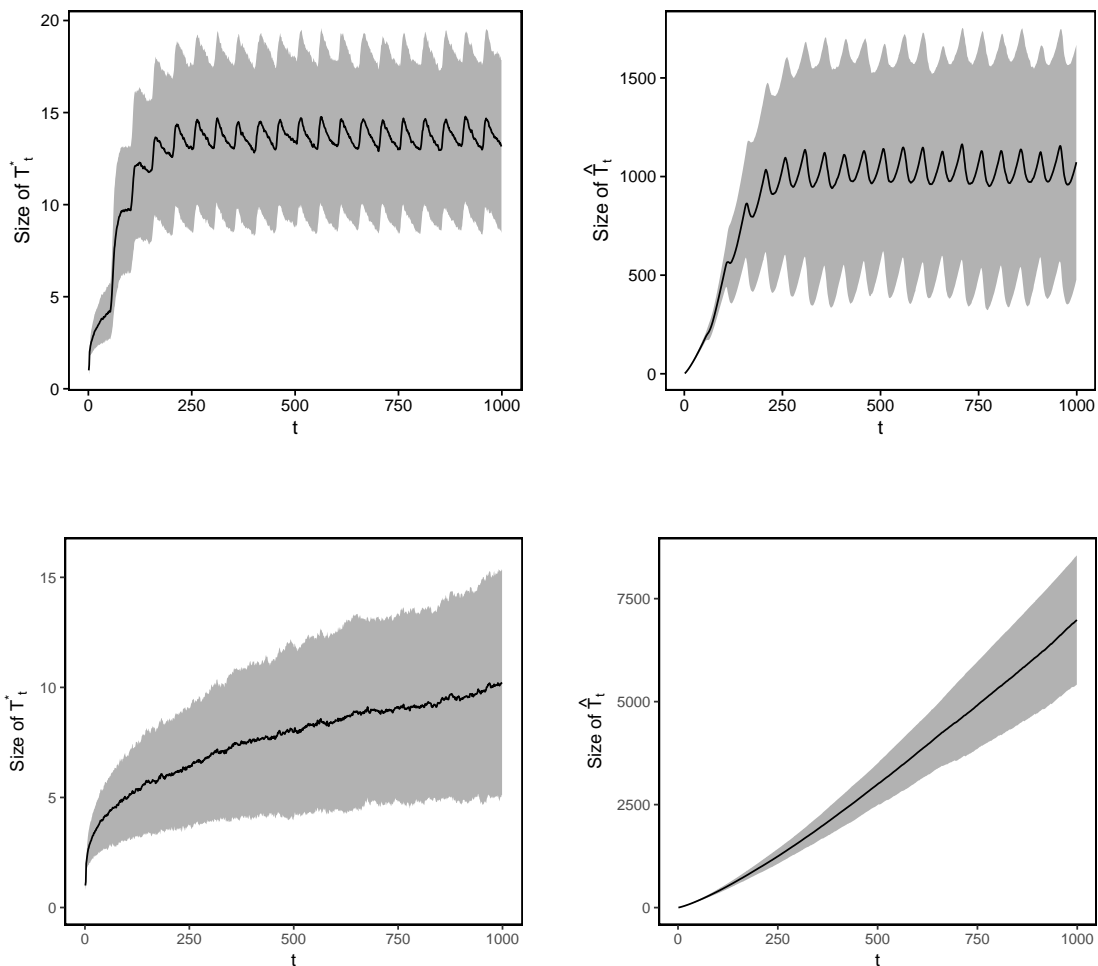


Figure 2: Size of  $\mathcal{T}_t^*$  (left-hand column) and  $\hat{\mathcal{T}}_t$  (right-hand column) as a function of  $t$  for data simulated with  $m = 19$  changepoints (top row) and no changepoints (bottom row). Lines show the average size, and shaded regions show plus or minus 1 standard deviation. Results are based on the analysis of 1000 data sets in each case.

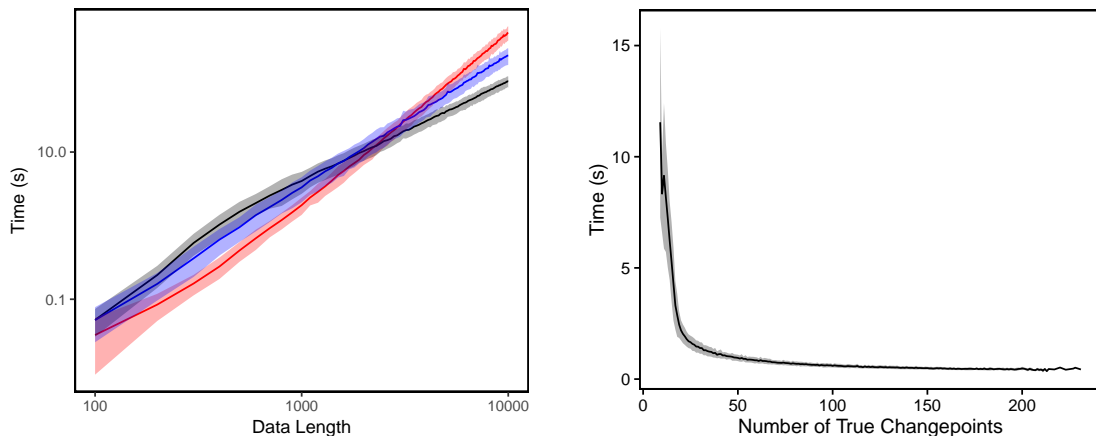


Figure 3: Computational cost, in seconds, of CPOP as we increase  $n$  (left-hand plot) and for fixed numbers of observations,  $n = 1000$ , but increasing numbers of changepoints (right-hand plot). For the former case we have used a log-scale on both axes, and we give average computational cost for three regimes for the number of changepoints,  $m$ : a fixed number of changepoints,  $m = 50$  (red); a linearly increasing number of changepoints,  $m = n/50$  (black); and  $m = \lfloor \sqrt{n} \rfloor$  (blue). Lines show the average computational cost, and shaded regions show plus or minus 1 standard deviation.

noise, binary segmentation would not correctly identify the changepoints.

To overcome this, Baranowski et al. (2016), present the *narrowest-over-threshold* algorithm, henceforth called the NOT algorithm. This algorithm proceeds by (i) taking a pre-specified number,  $M$ , of intervals of data,  $\mathbf{y}_{s_i:t_i}$  say; (ii) performing a generalised likelihood ratio test for a change in slope on each  $\mathbf{y}_{s_i:t_i}$ ; (iii) keeping all intervals for which the test-statistic is above some pre-specified threshold; (iv) ordering these intervals, with the shortest interval first and the longest last; (v) running down this list in order, adding changepoints at each of the inferred changepoint locations for an interval providing that interval does not contain any previously inferred changepoints. The idea of the algorithm is that by concentrating on the smallest intervals in (iv), these will be intervals that are likely to have at most one actual changepoint, and hence the inferred changepoint in step (v) should be close in position to this actual changepoint.

In practice, NOT is run for a continuous range of thresholds in step (iii). This will produce a set of different segmentations of the data. The segmentation that is then chosen is the one that minimises the BIC for a model where the residuals are independent Gaussian with unknown variance  $\sigma^2$ . For a segmentation with  $m$  changepoints at locations  $\boldsymbol{\tau}$ , the BIC corresponds to the minimum, over  $\boldsymbol{\phi}$  of

$$n \log \left( \frac{1}{n} \sum_{i=0}^m \left[ \sum_{t=\tau_i+1}^{\tau_{i+1}} \left( y_t - \frac{\phi_{\tau_{i+1}} - \phi_{\tau_i}}{\tau_{i+1} - \tau_i} (t - \tau_i) \right)^2 \right] \right) + 2m \log n.$$

This is closely related to our criterion (2) with the BIC penalty, except for the assumption of unknown variance, and the fact that this criterion is only minimised over the set of segmentations found by the NOT algorithm. One advantage of this approach is that it avoids the need to have an estimate of  $\sigma$ .

The other approach we compare to is the trend-filtering algorithm (Kim et al., 2009). Trend-filtering aims to minimise the residual sum of squares of the fitted continuous piecewise-linear mean, but with an  $L_1$  penalty on how the slope changes. Again, this is closely related to our criterion (2), except we use an  $L_0$  penalty on the changes in slope.

Trend-filtering requires a choice of penalty, in the same way that we need to choose the penalty  $\beta$  in (2). To mimic the approach of NOT we use a BIC type approach. This involves running the trend-filtering algorithm for a discrete set of penalty values. For a given penalty value, trend-filtering will output an estimate of the mean at each time point. From this we can infer the changepoint locations as the points where the estimated mean has a change in slope. We evaluate the output from each run of the trend-filtering algorithm using BIC. If the estimated mean is  $\hat{\phi}_{1:n}$ , and this has  $m$  changes in slope, then using the fact that for trend-filtering a segmentation with  $m$  changes in slope has an effective degrees of freedom that is  $m + 2$  (Tibshirani, 2014), the BIC value is

$$\frac{1}{\sigma^2} \left( \sum_{t=1}^n [y_t - \hat{\phi}_t]^2 \right) + (m + 2) \log(n).$$

Other approaches, including fitting a change in mean to differenced data and ignoring the continuity constraint when detecting changepoints, are considered in Maidstone (2016). However these all perform much worse, across all measures of accuracy, than the three approaches we compare here.

In the comparisons below we implement CPOP for minimising (2) with the BIC penalty. We use the `not` R-package to implement NOT, and the code available from [http://stanford.edu/~boyd/11\\_tf](http://stanford.edu/~boyd/11_tf) to implement trend-filtering. For NOT we set the number of intervals,  $M$  in step (i) of the algorithm above, to  $10^5$ . This is larger than recommended in Baranowski et al. (2016), but we found it gave slightly better results than the default choice of  $10^4$  intervals. For trend-filtering and CPOP we need an estimate of the variance of the residuals. Within a segment, the variance of the second differences of the data is easily shown to be 6 times the variance of the residuals. Thus we take second differences of the data, and take one-sixth of the median-absolute-deviation estimator of the variance of these second differences. Of course, being heuristic methods, both NOT and trend-filtering are much faster algorithms than CPOP. Across all the scenarios we considered, trend-filtering and NOT ran in a few seconds, whereas CPOP took between tens of seconds to a few minutes.

The three scenarios that we compared the methods on are shown in Figure 4. The first two of these, `wave1` and `wave2`, are taken from Baranowski et al. (2016). These two scenarios have a fixed

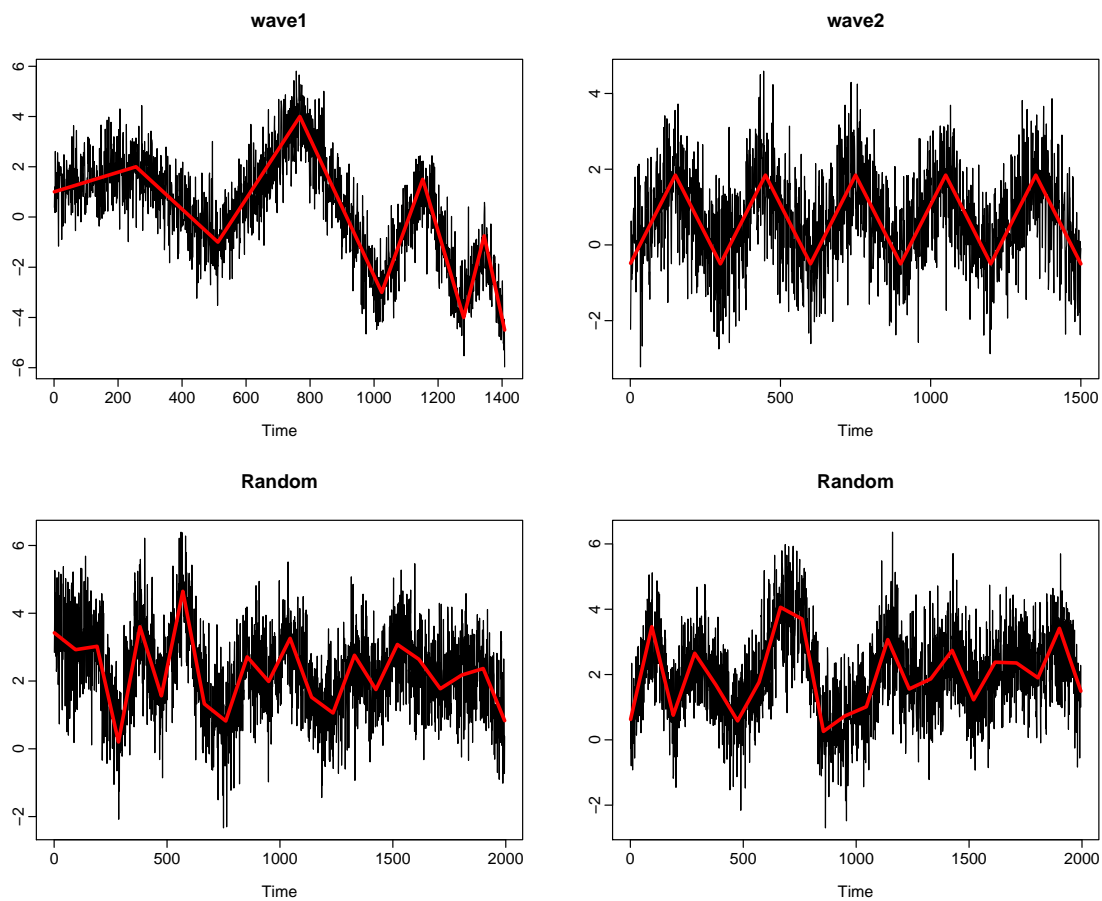


Figure 4: Example data from the three simulation scenarios we considered: **wave1** and **wave2** (top row) are taken from Baranowski et al. (2016) and the shape of the mean function is fixed in these scenarios. For the **Random** scenario (bottom row), the form of the mean is random, and we give two example realisations.

mean function. We consider extensions of these two scenarios with higher-frequency observations for **wave1**, where we have twice or four times as many observations within each segment; and longer time-series for **wave2**, where we have 20 or 40 segments, each of 150 observations, rather than just 10. In the third scenario, which we call **Random**, we simulate the underlying mean for each data set. This setting has segments of equal length, but the value of the mean function at the start/end of each segment is simulated from a Gaussian distribution with variance 4. For this setting we will consider varying both the number of data points and the number of changepoints. In all cases that data is obtained by adding independent standard Gaussian noise to the mean.

Following Baranowski et al. (2016), for **wave1** and **wave2** we compare methods using the mean square error (MSE) of the estimates of the mean, and using a scaled Hausdorff distance,  $d_H$ , to measure accuracy of the changepoint locations. This distance is defined as

$$d_H = \frac{1}{n_s} \max \left\{ \max_j \min_k |\tau_j - \hat{\tau}_k|, \max_k \min_j |\tau_j - \hat{\tau}_k| \right\},$$

where  $\hat{\tau}_k$  are the estimated changepoint locations,  $\tau_j$  the true changepoint locations, and  $n_s$  the length of the largest segment. The idea is that for each true change we find the closest estimated changepoint, and for each estimated changepoint we find the closest true changepoint. We then calculate the distance between each of these pairs of changepoints, and  $d_H$  is set to the largest of these distances divided by the length of the longest segment. The smaller  $d_H$  the better the estimates of the changepoints, with  $d_H = 0$  meaning that all changepoints are detected without error, and no other changepoints are estimated.

First we analyse data from the **wave1** and **wave2** scenarios. We consider different lengths of data with either a fixed number of changepoints (**wave1**) or with the number of changepoints increasing linearly with the number of data points (**wave2**). For both **wave1** and **wave2** there is a substantial change in the slope of the mean at each changepoint. As such, these represent relatively straightforward scenarios for detecting changepoints, and both NOT and CPOP perform well at detecting the number of changepoints: NOT correctly identifies the number of changepoints for all 600 simulated data sets, and CPOP correctly identifies the number of changepoints in over 99% of these cases. By comparison trend-filtering substantially over-estimates the number of changepoints in all cases. For **wave1** the average number of changes detected is 16 for  $n = 1408$ , rising to 29 for  $n = 5632$ , when the true number of changes is 7. We have similar over-estimation for **wave2**. The reason for this is the use the  $L_1$  penalty for the change in slope. The  $L_1$  penalty is the same for multiple consecutive changes in slope of the same sign as it is for one large change in slope. As a result trend-filtering tends to introduce multiple changepoints around each actual change.

This over-estimation of the number of changes results in the much larger value of  $d_H$  for this method than for NOT and CPOP: see the right-hand plots of Figure 5. Whilst NOT and CPOP perform



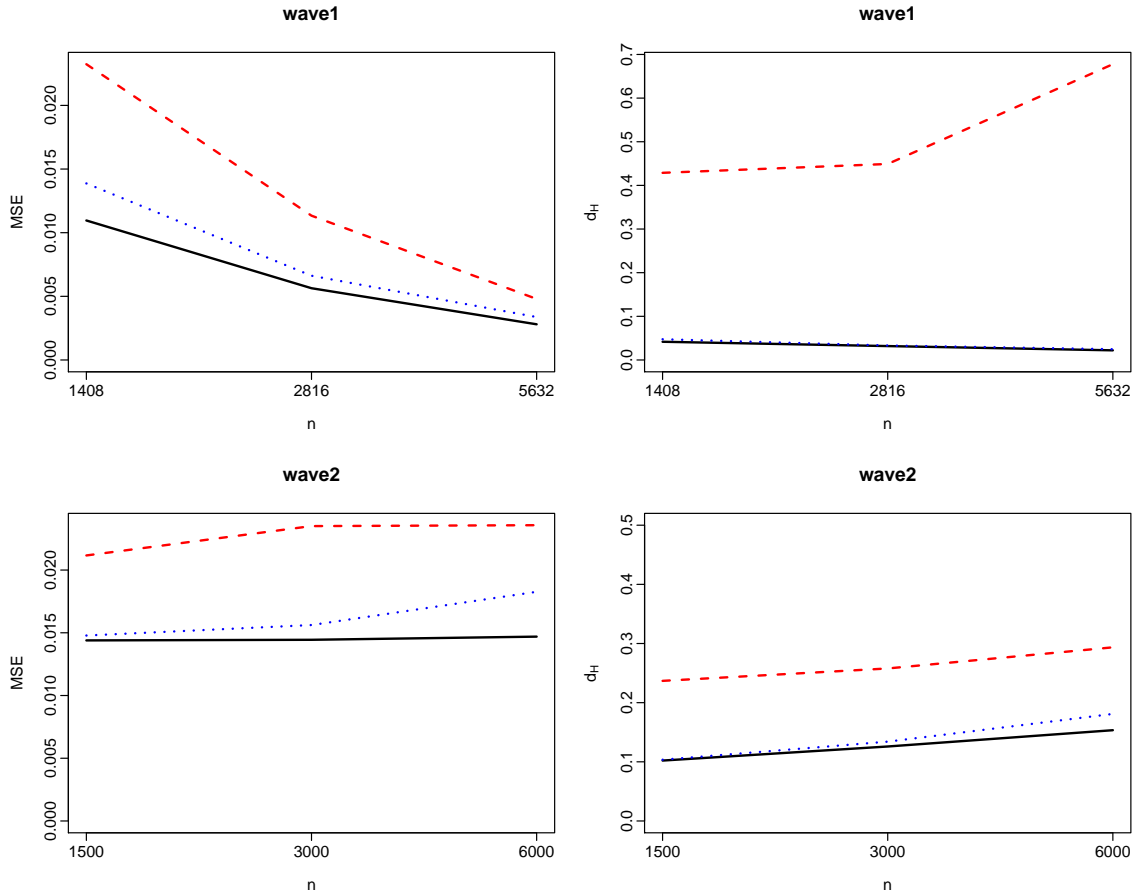


Figure 5: Results for CPOP (black solid line), NOT (blue dotted line) and trend-filtering (red dashed line) for **wave1** (top row) and **wave2** (bottom row). We give results for mean square error of the estimate of the mean (left-hand column) and for the accuracy of the estimates of the changepoint locations, measured via  $d_H$  (right-hand column). For **wave1** we considered data sets of length  $n = 1408$ ,  $n = 2816$  and  $n = 5632$ , each data set having 8 segments. For **wave2** we considered data sets of length  $n = 1500$ ,  $n = 3000$  and  $n = 6000$ , each data set having segments of length 150. Results are averaged over 100 data sets in for each scenario and each value of  $n$ .

similarly in terms of accuracy when estimating changepoint location, CPOP is more accurate in terms of estimating the underlying mean: see the MSE results in the left-hand plots of Figure 5. Again both methods perform better than trend-filtering. We believe the reason for this is that trend-filtering shrinks the change in slope towards 0. For signals like `wave1` and `wave2` where all changes in slope are substantial, this causes trend-filtering to under-estimate these changes. This can introduce substantial error at estimating the mean in regions around each changepoint.

We now compare the three methods on the `Random` simulation scenario. We consider data sets of length varying from 1000 to 10000, with either a fixed number of 20 segments or with the segment length fixed to 100. This is a harder scenario than either `wave1` or `wave2` as the change in slope differs considerably from changepoint to changepoint, with the change in slope being small in many cases (see the example data sets in the bottom row of Figure 4). As a result there are many changepoints that are hard to detect. In all cases CPOP and NOT under estimate the number of changes, while trend-filtering still over estimates this number. These two different sources of error are masked in the measure  $d_H$ , and thus we summarise the accuracy of changepoint detection through true-positive and false-positive proportions. To calculate these we say that an actual change is detected if there is an estimated changepoint within a certain distance of it. The results we show have set this distance to be a fifth of the segment length, though qualitatively similar results are obtained with different choices. We calculate the number of false positives as the number of changepoints detected less the number of true positives. Our results are in terms of the true-positive proportion, which is the proportion of actual changepoints detected, and the false-positive proportion, the proportion of detected the changepoints that are false-positive.

Results are shown in Figure 6. These are qualitatively different from the earlier results. For this problem we see that trend-filtering is most accurate in terms of estimating the underlying mean. We believe that trend-filtering is more suited to this scenario as there are a range of values for how much the slope changes at each changepoint, including many cases where the change is small. Hence the shrinking of the change in slope that trend-filtering induces is actually beneficial. As trend-filtering estimates more changes, it detects a higher proportion of true changepoints, but it has a high false-positive proportion: in all cases over 40% of the changepoints it finds are false-positives. By comparison both NOT and CPOP have lower false positive proportions, and encouragingly, this proportion decreases as the segment length increases (see top right-hand plot in Figure 6). Whilst NOT is marginally better in terms of accuracy of the detected changepoints, CPOP is substantially more accurate in terms of its estimate of the underlying mean.

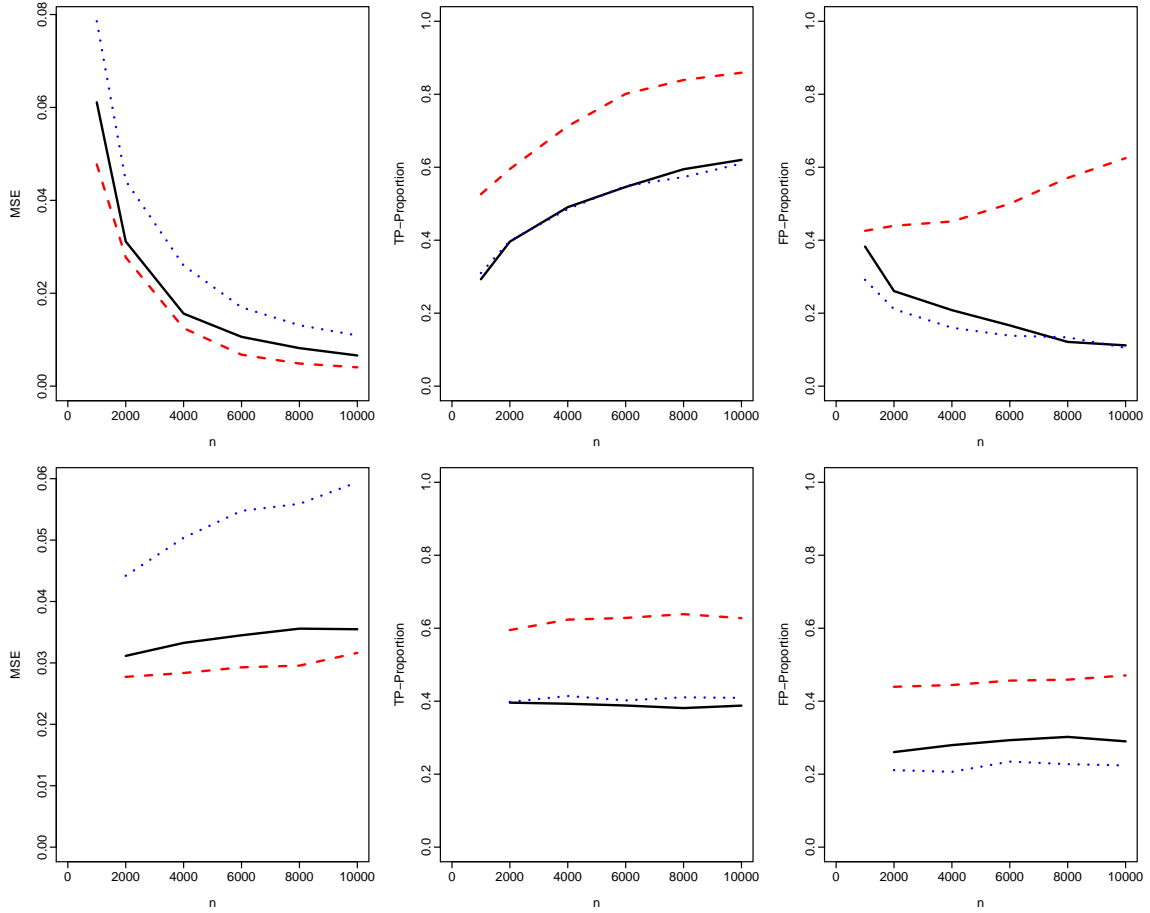


Figure 6: Results for CPOP (black solid line), NOT (blue dotted line) and trend-filtering (red dashed line) for the Random scenario with a fixed number of changepoints (top row) and a fixed segment length (bottom row). We give results for mean square error of the estimate of the mean (left-hand column) and for the accuracy of the estimates of the changepoint locations, measured via the proportion of true-positives (middle column) and of false-positives (right-hand column). For the top row we have 20 segments for each data set, for the bottom row we have segments of length 100 for each data set. Results are averaged over 100 data sets for each case and each value of  $n$ .

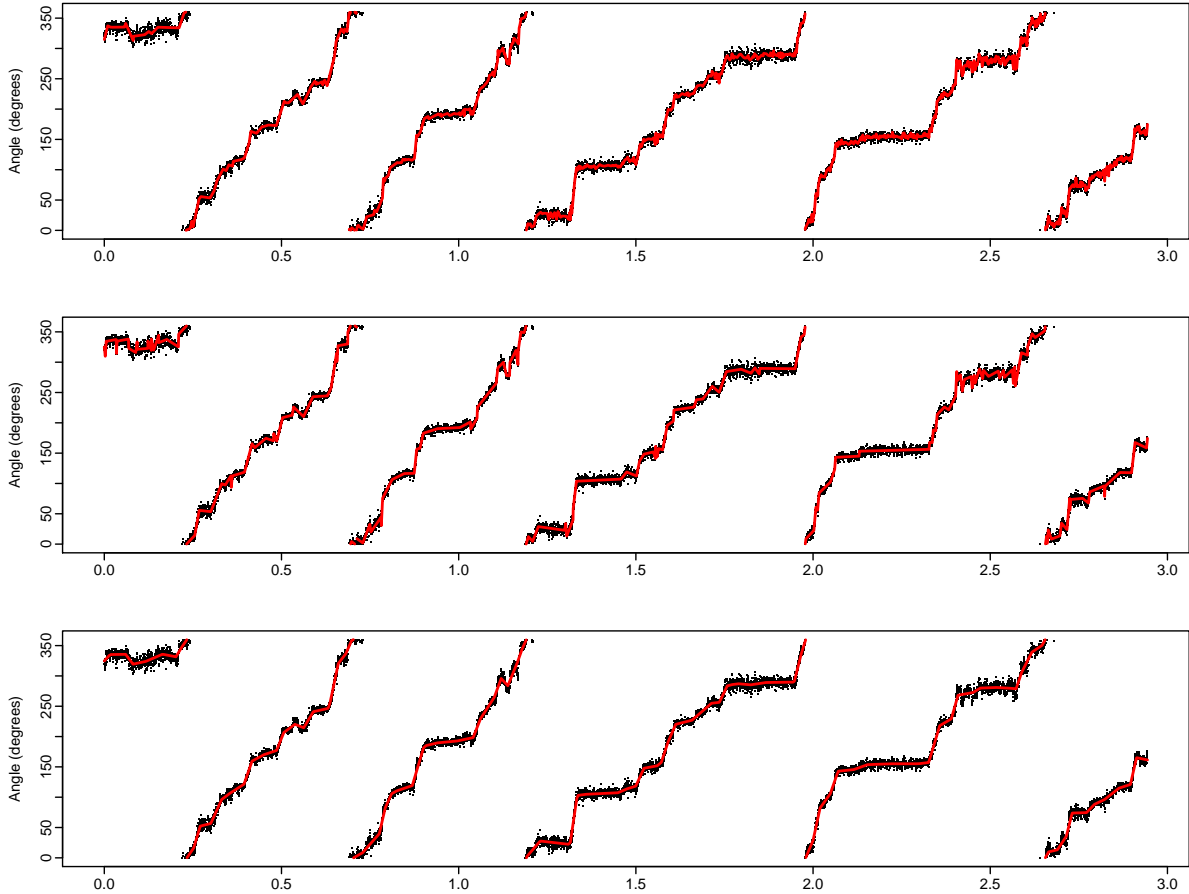


Figure 7: Time-series of angular position (data from Sowa et al., 2005) and example fits obtained by NOT (top); CPOP (middle) and trend-filtering (bottom). The fit obtained by CPOP is the one that contains the same number, 182, of changepoints as that found by NOT (see text for more details). For ease of presentation we have plotted the angle of the bacteria, the model we fit assumes continuity of angles of 360 degrees (top of each plot) and 0 degrees (bottom of each plot).

## 5 Bacterial Flagella Motor Data

We return to the bacterial flagella motor data we introduced in Section 1 and Figure 1. For more background on these biological systems see (Sowa et al., 2005; Sowa and Berry, 2008; Zhou et al., 1998). Data similar to those we analyse has been collected by Ryu et al. (2000); Chen and Berg (2000a,b); Sowa et al. (2003) among others. Here we look at how well we can extract the angular motion by fitting changepoint models, and in particular change-in-slope models using the CPOP algorithm. The data we analyse comes from Sowa et al. (2005) and is shown in Figure 7. It consists of 11,912 observations.

The aim of our analysis is to fit the underlying angular position. We first compared fitting a continuous piecewise linear mean to both fitting a piecewise constant mean and a discontinuous

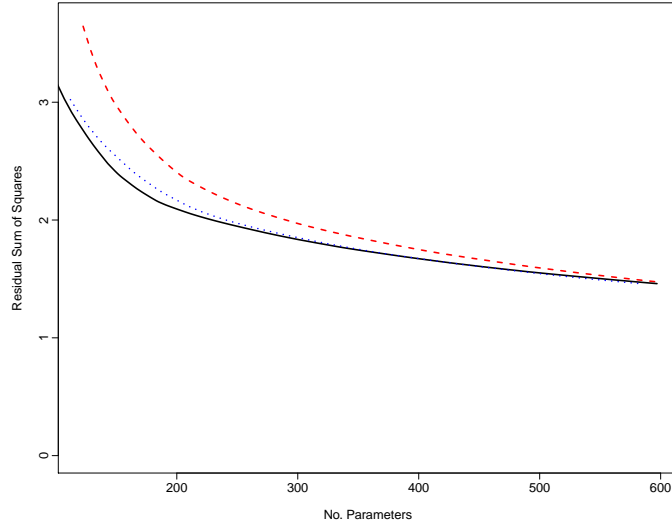


Figure 8: Accuracy of fits of data shown in Figure 7 by a piecewise constant mean (red dashed line), a continuous piecewise-linear mean (black full line) and a discontinuous piecewise-linear mean (blue dotted line). For each type of line we found the best segmentation, in terms of minimising the residual sum of squares (RSS) of the fit, for a range of the number of changepoints. We plot the RSS against the number of free parameters of the fitted mean function for each case.

piecewise linear mean. We fit the latter two by minimising the residual sum of squares plus a penalty times the number of changepoints, using the PELT algorithm (Killick et al., 2012). In all cases we varied the penalty value using the CROPS algorithm (Haynes et al., 2016). Different penalty values lead to optimal segmentations with different numbers of changepoints. For each different segmentation we calculated the actual residual sum of squares of the fit we obtained. A plot of this against the number of free parameters in the fitted mean is shown in Figure 8. We can see that fitting a continuous piecewise-linear function, which is more natural for this application, leads to a uniformly better fit to the data than the change in mean for any given number of parameters. The assumption of continuity also gives improvements for fitted means with fewer than 400 parameters. While the differences in residual sum of squares looks small, due to the large number of observations, the reduction in log-likelihood, under a model where the residuals are iid Gaussian, is still substantial. For example, for models with fewer than 350 parameters, the best fitting continuous mean has a log-likelihood that is 32.4 units greater than the best fitting discontinuous mean.

We also compared the accuracy of using CPOP to analyse this data to that of using NOT and trend-filtering. A comparison of the fits obtained using NOT, CPOP and trend-filtering are shown in Figure 7. We ran NOT with a total of  $10^6$  random intervals, and have plotted the segmentation that minimised the SIC. This segmentation has 794 changepoints, largely because it substantially

overfits the latter part of the data. For comparison, an example fit from CPOP is also shown. The segmentation obtained using CPOP has 182 changepoints. Despite fewer changes, it has a smaller residual sum of squares than the segmentation that NOT found: 1.72 as compared to 1.80.

We also ran trend-filtering for a range of penalty values. For all penalty values that gave a reasonable fit to the data, the number of changes in slope was large: with changes at more than half the time-points. In these cases the majority of changes in slope were small. As a crude approach to choosing a sensible segmentation we defined there to be a change-point if the change in slope was non-zero after rounding to 3 decimal places. Using this definition we then found the segmentation that minimised the SIC. This is shown in the bottom plot of 8. This had 278 changepoints under our definition, and 10,850 actual changes in slope. We see that the estimated mean we obtained appears to under-fit the data in a number of places. It has a higher residual sum of squares, 2.94, than the fitted mean shown for either CPOP or NOT.

## 6 Discussion

We have presented a continuous-state dynamic programming algorithm for finding the best continuous piecewise linear fit to data under a criterion that measures fit to the data using the residual sum of squares and penalises complexity through the number of changes in slope. This is a setting where standard dynamic programming approaches for changepoint detection do not work, due to the dependence across segments imposed by the continuity constraint. Empirically this approach is feasible for data with up to 10,000 data points and 100s of changepoints. For such challenging scenarios, we see from the analysis of the bacterial flagella motor data, that this method can produce a substantially better fit to the data than faster approximate alternatives like NOT and trend-filtering.

The dynamic programming approach we have used has the potential to be applied to a much wider range of changepoint problems with dependence across segments. The key requirement is that we can construct a recursion for a set of functions, our  $f^t(\phi)$ , that are piecewise quadratic in some univariate parameter  $\phi$ . This requires that we measure fit to the data through the residual sum of squares, that the dependence of the parameters in successive segments is through a univariate quantity  $\phi$ , and that any constraints on parameters in successive segments respect the piecewise quadratic nature of  $f^t(\phi)$ . This would cover change in mean or slope under monotonicity constraints, our change in slope model with an additional  $L_1$  or  $L_2$  penalty on the change in slope, or more general models for the mean that are piecewise polynomial and continuous.

The requirement that dependence across segments is through a univariate quantity comes from our

functional pruning approach. Such pruning is important for reducing the computational complexity of the algorithm. It is unclear whether functional pruning can be implemented for piecewise quadratic functions,  $f^t(\phi)$ , when  $\phi$  is not univariate as the line search approach we take does not generalise beyond the univariate case. Even if not, it may be possible to develop efficient algorithms that implement an approximate version of functional pruning.

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## References

- Aston, J. A. and Kirch, C. (2012). Evaluating stationarity via change-point alternatives with applications to fmri data. *The Annals of Applied Statistics*, pages 1906–1948.
- Baranowski, R., Chen, Y., and Fryzlewicz, P. (2016). Narrowest-Over-Threshold Detection of Multiple Change-points and Change-point-like Features. *ArXiv:1609.00293*.
- Chen, X. and Berg, H. C. (2000a). Solvent-isotope and pH effects on flagellar rotation in *Escherichia coli*. *Biophysical journal*, 78(5):2280–2284.
- Chen, X. and Berg, H. C. (2000b). Torque-speed relationship of the flagellar rotary motor of *Escherichia coli*. *Biophysical Journal*, 78(2):1036–1041.
- Davis, R. A., Lee, T. C. M., and Rodriguez-Yam, G. A. (2006). Structural break estimation for nonstationary time series models. *Journal of the American Statistical Association*, 101:223–239.
- Fryzlewicz, P. (2014). Wild binary segmentation for multiple change-point detection. *The Annals of Statistics*, 42(6):2243–2281.
- Futschik, A., Hotz, T., Munk, A., and Sieling, H. (2014). Multiscale DNA partitioning: statistical evidence for segments. *Bioinformatics*, page btu180.
- Goldberg, N., Kim, Y., Leyffer, S., and Veselka, T. D. (2014). Adaptively refined dynamic program for linear spline regression. *Computational Optimization and Applications*, 58(3):523–541.
- Hampel, F. R. (1974). The influence curve and its role in robust estimation. *Journal of the American Statistical Association*, 69(346):383–393.

- Haynes, K., Eckley, I. A., and Fearnhead, P. (2016). Computationally efficient changepoint detection for a range of penalties. *Journal of Computational and Graphical Statistics*, To appear.
- Hocking, T. D., Boeva, V., Rigaiil, G., Schleiermacher, G., Janoueix-Lerosey, I., Delattre, O., Richer, W., Bourdeaut, F., Suguro, M., Seto, M., Bach, F., and Vert, J.-P. (2014). SegAnnDB: interactive web-based genomic segmentation. *Bioinformatics*, 30:1539–46.
- Horner, A. and Beauchamp, J. (1996). Piecewise-linear approximation of additive synthesis envelopes : a comparison of various methods. *Computer Music Journal*, 20(2):72–95.
- Hotz, T., Schtte, O. M., Sieling, H., Polupanow, T., Diederichsen, U., Steinem, C., and Munk, A. (2013). Idealizing ion channel recordings by a jump segmentation multiresolution filter. *IEEE Transactions on NanoBioscience*, 12(4):376–386.
- Jackson, B., Scargle, J. D., Barnes, D., Arabhi, S., Alt, A., Gioumousis, P., Gwin, E., Sangtrakulcharoen, P., Tan, L., and Tsai, T. T. (2005). An algorithm for optimal partitioning of data on an interval. *IEE Signal Processing Letters*, 12:105–108.
- Killick, R., Eckley, I. A., Ewans, K., and Jonathan, P. (2010). Detection of changes in variance of oceanographic time-series using changepoint analysis. *Ocean Engineering*, 37(13):1120–1126.
- Killick, R., Fearnhead, P., and Eckley, I. A. (2012). Optimal detection of changepoints with a linear computational cost. *Journal of the American Statistical Association*, 107:1590–1598.
- Kim, S. J., Koh, K., Boyd, S., and Gorinevsky, D. (2009).  $l_1$  Trend Filtering. *SIAM Review*, 51(2):339–360.
- Lavielle, M. and Moulines, E. (2000). Least-squares estimation of an unknown number of shifts in a time series. *Journal of time series analysis*, 21(1):33–59.
- Maidstone, R. (2016). *Efficient analysis of complex changepoint problems*. PhD thesis, Lancaster University.
- Maidstone, R., Hocking, T., Rigaiil, G., and Fearnhead, P. (2017). On optimal multiple changepoint algorithms for large data. *To appear in Statistics and Computing*.
- National Research Council (2013). *Frontiers in massive data analysis*.
- Nemeth, C., Fearnhead, P., and Mihaylova, L. (2014). Sequential Monte Carlo Methods for State and Parameter Estimation in Abruptly Changing Environments. *IEEE Transactions on Signal Processing*, 62(5):1245–1255.



- Rigaill, G. (2015). A pruned dynamic programming algorithm to recover the best segmentations with 1 to  $K_{\max}$  change-points. *Journal de la Société Française de Statistique*, 156(4):180–205.
- Ryu, W. S., Berry, R. M., and Berg, H. C. (2000). Torque-generating units of the flagellar motor of *Escherichia coli* have a high duty ratio. *Nature*, 403:444–447.
- Schwarz, G. (1978). Estimating the dimension of a model. *The Annals of Statistics*, 6(2):461–464.
- Scott, A. J. and Knott, M. (1974). A cluster analysis method for grouping means in the analysis of variance. *Biometrics*, 30:507–512.
- Sowa, Y. and Berry, R. M. (2008). Bacterial flagellar motor. *Quarterly Reviews of Biophysics*, 41(02):103–132.
- Sowa, Y., Hotta, H., Homma, M., and Ishijima, A. (2003). Torque-speed relationship of the Na<sup>+</sup>-driven flagellar motor of *Vibrio alginolyticus*. *Journal of Molecular Biology*, 327(5):1043–1051.
- Sowa, Y., Rowe, A., Leake, M., Yakushi, T., Homma, M., Ishijima, A., and Berry, R. (2005). Direct observation of steps in rotation of the bacterial flagellar motor. *Nature*, 437(7060):916–9.
- Tibshirani, R. J. (2014). Adaptive piecewise polynomial estimation via trend filtering. *The Annals of Statistics*, 42(1):285–323.
- Tomé, A. R. and Miranda, P. M. A. (2004). Piecewise linear fitting and trend changing points of climate parameters. *Geophysical Research Letters*, 31(2).
- Weinmann, A. and Storath, M. (2015). Iterative Potts and Blake–Zisserman minimization for the recovery of functions with discontinuities from indirect measurements. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 471(2176).
- Yao, Y.-C. (1988). Estimating the number of change-points via Schwarz’ criterion. *Statistics & Probability Letters*, 6(3):181–189.
- Zhang, N. R. and Siegmund, D. O. (2007). A modified Bayes information criterion with applications to the analysis of comparative genomic hybridization data. *Biometrics*, 63:22–32.
- Zhou, J., Lloyd, S. A., and Blair, D. F. (1998). Electrostatic interactions between rotor and stator in the bacterial flagellar motor. *Proceedings of the National Academy of Sciences of the United States of America*, 95(May):6436–6441.

## Appendix A Updates for Quadratic Functions

In Section 3 (equation 6) we define a function,  $f_{\tau}^t(\phi)$ , as the minimum cost of segmenting  $\mathbf{y}_{1:t}$  with changepoints at  $\tau = \tau_1, \dots, \tau_k$  and fitted value  $\phi_t = \phi$  at time  $t$ . We then derived a recursion for these functions as follows

$$f_{\tau}^t(\phi) = \min_{\phi'} \left\{ f_{\tau_1, \dots, \tau_{k-1}}^{\tau_k}(\phi') + \mathcal{C}(y_{\tau_k+1:t}, \phi', \phi) + \beta + h(\tau_{i+1} - \tau_i) \right\}. \quad (14)$$

The functions  $f_{\tau}^t(\phi)$  are quadratics in  $\phi$ , and we denote  $f_{\tau}^t(\phi)$  as follows

$$f_{\tau}^t(\phi) = a_{\tau}^t + b_{\tau}^t \phi + c_{\tau}^t \phi^2, \quad (15)$$

for some constants  $a_{\tau}^t$ ,  $b_{\tau}^t$  and  $c_{\tau}^t$ . We then wish to calculate these coefficients by updating the coefficients that make up  $f_{\tau_1, \dots, \tau_{k-1}}^{\tau_k}(\phi')$  using (14). To do this we need to write the cost for the segment from  $\tau_k + 1$  to  $t$  in quadratic form. Defining the length of the segment as  $s = t - \tau_k$  this cost can be written as

$$\begin{aligned} \mathcal{C}(y_{\tau_k+1:t}, \phi', \phi) &= \frac{(s+1)(2s+1)}{6s\sigma^2} \phi^2 + \left( \frac{(s+1)}{\sigma^2} - \frac{(s+1)(2s+1)}{3s\sigma^2} \right) \phi' \phi \\ &\quad - \left( \frac{2}{s\sigma^2} \sum y_j(j - \tau_k) \right) \phi + \left( \frac{1}{\sigma^2} \sum y_i^2 \right) \\ &\quad + 2 \left( \frac{1}{s\sigma^2} \sum y_j(j - \tau_k) - \frac{1}{\sigma^2} \sum y_i \right) \phi' + \frac{(s-1)(2s-1)}{6s\sigma^2} \phi'^2. \end{aligned} \quad (16)$$

Writing (16) as  $A\phi^2 + B\phi'\phi + C\phi + D + E\phi' + F\phi'^2$  for constants  $A, B, C, D$  and  $E$ , substituting (16) into (14) and minimising out  $\phi'$  we can get the formula for the updating the coefficients of the quadratic  $f_{\tau}^t(\phi)$ :

$$\begin{aligned} a_{\tau}^t &= A - \frac{B^2}{4 \left( a_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + F \right)}, \\ b_{\tau}^t &= C - \frac{\left( b_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + E \right) B}{2 \left( a_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + F \right)}, \\ c_{\tau}^t &= c_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + D - \frac{\left( b_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + E \right)^2}{4 \left( a_{(\tau_1, \dots, \tau_{k-1})}^{\tau_k} + F \right)} + \beta + h(t - \tau_k). \end{aligned} \quad (17)$$

## Appendix B Proofs

### B.1 Proof of Theorem 3.1

The proof of Theorem 3.1 works by contrapositive. We show that if  $(\boldsymbol{\tau}, s) \in \mathcal{T}_t^*$  then a necessary condition of this is that  $\boldsymbol{\tau} \in \mathcal{T}_s^*$ , taking the contrapositive of this gives Theorem 3.1.

**Proof.** Assume  $(\boldsymbol{\tau}, s) \in \mathcal{T}_t^*$ , then there exists  $\phi$  such that

$$f^t(\phi) = f_{(\boldsymbol{\tau}, s)}^t(\phi),$$

Now for any  $\phi^*$ ,

$$\begin{aligned} f^s(\phi^*) + \mathcal{C}(\mathbf{y}_{s+1:t}, \phi^*, \phi) + \beta &\geq \min_{\phi', r} [f^r(\phi') + \mathcal{C}(\mathbf{y}_{r+1:t}, \phi', \phi) + \beta], \\ &= f^t(\phi), \\ &= f_{(\boldsymbol{\tau}, s)}^t(\phi), \\ &= \min_{\phi''} \{f_{\boldsymbol{\tau}}^s(\phi'') + \mathcal{C}(\mathbf{y}_{s+1:t}, \phi'', \phi) + \beta\}, \\ &= f_{\boldsymbol{\tau}}^s(\phi^A) + \mathcal{C}(\mathbf{y}_{s+1:t}, \phi^A, \phi) + \beta, \end{aligned} \tag{18}$$

where  $\phi^A$  is the value of  $\phi''$  which minimises (18). As  $\phi^*$  can be chosen as any value, we can choose it as  $\phi^A$ . By cancelling terms we get  $f^s(\phi^A) \geq f_{\boldsymbol{\tau}}^s(\phi^A)$  and hence (from (7)),  $f^s(\phi^A) = f_{\boldsymbol{\tau}}^s(\phi^A)$  and therefore  $\boldsymbol{\tau} \in \mathcal{T}_s^*$ . We have shown that if  $(\boldsymbol{\tau}, s) \in \mathcal{T}_t^*$  then  $\boldsymbol{\tau} \in \mathcal{T}_s^*$ , by taking the contrapositive the theorem holds.  $\blacksquare$

### B.2 Proof of Theorem 3.2

The proof for Theorem 3.2 follow a similar argument to the corresponding proof in Killick et al. (2012). However we have to add a segment consisting of the single point  $y_{t+1}$  to deal with the dependence between the segments.

**Proof.** Let  $\boldsymbol{\tau}^*$  denote the optimal segmentation of  $\mathbf{y}_{1:t}$ . First consider  $T = t + 1$ . As adding a changepoint without penalty will always reduce the cost, it is straightforward to show

$$\begin{aligned} f_{\boldsymbol{\tau}^*}^T(\phi) &\geq \min_{\phi'} [f_{\boldsymbol{\tau}^*}^t(\phi') + \mathcal{C}(y_{t+1}, \phi', \phi)], \\ &= \min_{\phi'} [f_{\boldsymbol{\tau}^*}^t(\phi')] + \min_{\phi'} [\mathcal{C}(y_{t+1}, \phi', \phi)], \\ &> \min_{\phi'} [f^t(\phi')] + K + \min_{\phi'} [\mathcal{C}(y_{t+1}, \phi', \phi)], \\ &\geq \min_{\phi'} [f^t(\phi') + \mathcal{C}(y_{t+1}, \phi') + \beta + h(1)]. \end{aligned}$$

Thus segmenting  $\mathbf{y}_{1:T}$  with changepoints  $\boldsymbol{\tau}$  always has a greater cost than segmenting  $\mathbf{y}_{1:T}$  with changepoints  $(\boldsymbol{\tau}^*, t)$ .

Now we consider  $T > t + 1$ . We start by noting that by adding changes, at any point, without the penalty term and minimising over the corresponding  $\phi$  values will also decrease the cost. Therefore we have

$$f_{\boldsymbol{\tau}}^T(\phi) \geq \min_{\phi', \phi''} [f_{\boldsymbol{\tau}}^t(\phi') + \mathcal{C}(y_{t+1}, \phi', \phi'') + \mathcal{C}(\mathbf{y}_{t+2:T}, \phi'', \phi)]. \quad (19)$$

Then assuming that (13) is true, it can be shown that the segmenting the data  $\mathbf{y}_{1:T}$  with changepoints  $\boldsymbol{\tau}$  is always sub-optimal.

So from (19) and using (13),

$$\begin{aligned} f_{\boldsymbol{\tau}}^T(\phi) &\geq \min_{\phi', \phi''} [f_{\boldsymbol{\tau}}^t(\phi') + \mathcal{C}(y_{t+1}, \phi', \phi'') + \mathcal{C}(\mathbf{y}_{t+2:T}, \phi'', \phi)], \\ &\geq \min_{\phi'} [f_{\boldsymbol{\tau}}^t(\phi')] + \min_{\phi', \phi''} [\mathcal{C}(y_{t+1}, \phi', \phi'') + \mathcal{C}(\mathbf{y}_{t+2:T}, \phi'', \phi)], \\ &> \min_{\phi'} [f^t(\phi')] + K + \min_{\phi', \phi''} [\mathcal{C}(y_{t+1}, \phi', \phi'') + \mathcal{C}(\mathbf{y}_{t+2:T}, \phi'', \phi)], \\ &\geq \min_{\phi', \phi''} [f^t(\phi') + \mathcal{C}(y_{t+1}, \phi', \phi'') + \beta + h(1) + \mathcal{C}(\mathbf{y}_{t+2:T}, \phi'', \phi) + \beta + h(T - t + 1)]. \end{aligned}$$

The last step is due to the cost on a single point,  $\mathcal{C}(y_t, \phi', \phi'')$  only depending on  $\phi''$ , and by using the definition of  $K$ .

Therefore the cost of segmenting  $\mathbf{y}_{1:T}$  with changepoints  $\boldsymbol{\tau}$  is always greater than the cost of segmenting  $\mathbf{y}_{1:T}$  with changepoints  $(\boldsymbol{\tau}^*, t, t + 1)$  (where  $\boldsymbol{\tau}^*$  is the optimal segmentation of  $\mathbf{y}_{1:t}$ ) and this holds for all  $T > t + 1$  and hence  $\boldsymbol{\tau}$  can be pruned.  $\blacksquare$

## Appendix C Pseudo-Code for CPOP

The CPOP algorithm uses Algorithm 2 to calculate the intervals on which each function is optimal. This then enables the functions that are not optimal for any value of  $\phi$  to be removed. The idea of this algorithm is as follows.

We initialise the algorithm by setting the current parameter value as  $\phi_{curr} = -\infty$  and comparing the cost functions in our current set of candidates (which we initialise as  $\mathcal{T}_{temp} = \hat{\mathcal{T}}_t$ ) to get the optimal segmentation for this value,  $\boldsymbol{\tau}_{curr}$ . For each  $\boldsymbol{\tau} \in \mathcal{T}_{curr}$  we calculate where  $f_{\boldsymbol{\tau}}^t$  next intercepts with  $f_{\boldsymbol{\tau}_{curr}}^t$  (smallest value of  $\phi$  for which  $f_{\boldsymbol{\tau}}^t(\phi) = f_{\boldsymbol{\tau}_{curr}}^t(\phi)$  and  $\phi > \phi_{curr}$ ) and store this as  $x_{\boldsymbol{\tau}}$ . If for a  $\boldsymbol{\tau} \in \mathcal{T}_{temp}$  we have  $x_{\boldsymbol{\tau}} = \emptyset$  (i.e.  $f_{\boldsymbol{\tau}}^t$  doesn't intercept with  $f_{\boldsymbol{\tau}_{curr}}^t$  for any  $\phi > \phi_{curr}$ ) then we remove  $\boldsymbol{\tau}$  from  $\mathcal{T}_{temp}$ . We take the minimum of  $x_{\boldsymbol{\tau}}$  (the first of the intercepts) and set it as our new  $\phi_{curr}$  and the corresponding changepoint vector that produces it as  $\boldsymbol{\tau}_{curr}$ . We repeat this procedure

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**Algorithm 1:** Algorithm for Continuous Piecewise-linear Optimal Partitioning (CPOP)

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**Input** : Set of data of the form  $\mathbf{y}_{1:n} = (y_1, \dots, y_n)$ .

A positive penalty constant,  $\beta$ , and a non-negative, non-decreasing penalty function  $h(\cdot)$ .

Let  $n = \text{length of data}$ ;

set  $\hat{\mathcal{T}}_1 = \{0\}$ ;

and set  $K = 2\beta + h(1) + h(n)$ ;

**for**  $t = 1, \dots, n$  **do**

**for**  $\tau \in \hat{\mathcal{T}}_t$  **do**

**if**  $\tau = \{0\}$  **then**

$$\left[ \begin{array}{l} f_{\tau}^t(\phi) = \min_{\phi'} \mathcal{C}(\mathbf{y}_{1:t}, \phi', \phi) + h(t); \end{array} \right.$$

**else**

$$\left[ \begin{array}{l} f_{\tau}^t(\phi) = \min_{\phi'} \left\{ f_{\tau_1, \dots, \tau_{k-1}}^{\tau_k}(\phi') + \mathcal{C}(\mathbf{y}_{\tau_k+1:t}, \phi', \phi) + h(t - \tau_k) + \beta \right\}; \end{array} \right.$$

**for**  $\tau \in \hat{\mathcal{T}}_t$  **do**

$$\left[ \begin{array}{l} \text{Int}_{\tau}^t = \left\{ \phi : f_{\tau}^t(\phi) = \min_{\tau' \in \hat{\mathcal{T}}_t} f_{\tau'}^t(\phi) \right\}; \end{array} \right.$$

$$\left[ \begin{array}{l} \mathcal{T}_t^* = \{ \tau : \text{Int}_{\tau}^t \neq \emptyset \}; \end{array} \right.$$

$$\left[ \begin{array}{l} \hat{\mathcal{T}}_{t+1} = \hat{\mathcal{T}}_t \cup \left\{ (\tau, t) : \tau \in \mathcal{T}_t^* \right\}; \end{array} \right.$$

$$\left[ \begin{array}{l} \hat{\mathcal{T}}_{t+1} = \left\{ \tau \in \hat{\mathcal{T}}_{t+1} : \min_{\phi} f_{\tau}^t(\phi) \leq \min_{\phi', \tau'} [f_{\tau'}^t(\phi')] + K \right\}; \end{array} \right.$$

$$f_{opt} = \min_{\tau, \phi} f_{\tau}^n(\phi);$$

$$\tau_{opt} = \arg \min_{\tau} \left[ \min_{\phi} f_{\tau}^n(\phi) \right];$$

**Output:** The optimal cost,  $f_{opt}$ , and the corresponding changepoint vector,  $\tau_{opt}$ .

---

until the set  $\mathcal{T}_{temp}$  consists of only a single value  $\tau_{curr}$  which is the optimal segmentation for all future  $\phi > \phi_{curr}$ .

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**Algorithm 2:** Algorithm for calculation of  $Int_{\tau}^t$  at time  $t$

---

**Input** : Set of changepoint candidate vectors  $\hat{\mathcal{T}}_t$  for current timestep,  $t$ ,  
Optimal segmentation functions  $f_{\tau}^t(\phi)$  for current time step  $t$  and  $\tau \in \hat{\mathcal{T}}_t$ .

$$\mathcal{T}_{temp} = \hat{\mathcal{T}}_t;$$

$$Int_{\tau}^t = \emptyset \text{ for } \tau \in \hat{\mathcal{T}}_t;$$

$$\phi_{curr} = -\infty;$$

$$\tau_{curr} = \arg \min_{\tau \in \mathcal{T}_{temp}} [f_{\tau}^t(\phi_{curr})];$$

**while**  $\mathcal{T}_{temp} \setminus \{\tau_{curr}\} \neq \emptyset$  **do**

**for**  $\tau \in \mathcal{T}_{temp} \setminus \{\tau_{curr}\}$  **do**

$$\quad x_{\tau} = \min\{\phi : f_{\tau}^t(\phi) - f_{\tau_{curr}}^t(\phi) = 0 \ \& \ \phi > \phi_{curr}\};$$

**if**  $x_{\tau} = \emptyset$  **then**

$$\quad \quad \mathcal{T}_{temp} = \mathcal{T}_{temp} \setminus \{\tau\}$$

$$\tau_{new} = \arg \min_{\tau} (x_{\tau});$$

$$\phi_{new} = \min_{\tau} (x_{\tau});$$

$$Int_{\tau_{curr}}^t = [\phi_{curr}, \phi_{new}] \cup Int_{\tau_{curr}}^t;$$

$$\tau_{curr} = \tau_{new};$$

$$\phi_{curr} = \phi_{new};$$

**Output:** The intervals  $Int_{\tau}^t$  for  $\tau \in \hat{\mathcal{T}}_t$

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