

PeakSegDisk usage examples

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Welcome to PeakSegDisk, an R package for optimal peak detection in very large count data sequences.

1 Related work

The PeakSeg R packages contain algorithms for inferring optimal segmentation models subject to the constraint that up changes must be followed by down changes, and vice versa. This ensures that the model can be interpreted in terms of peaks (after up changes) and background (after down changes).

PeakSegDP the historically first PeakSeg package, <https://CRAN.R-project.org/package=PeakSegDP> provides a heuristic quadratic time algorithm for computing models from 1 to S segments for a single sample. This was the original algorithm described in our ICML'15 paper, <http://jmlr.org/proceedings/papers/v37/hocking15.html>, but it is neither fast nor optimal, so in practice we recommend to use our newer packages below instead.

PeakSegOptimal <https://CRAN.R-project.org/package=PeakSegOptimal> provides log-linear time algorithms for computing optimal models with multiple peaks for a single sample. The algorithms are faster and more accurate than PeakSegDP. Citation: JMLR'20, <https://jmlr.org/papers/v21/18-843.html>

PeakSegDisk <https://github.com/tdhock/PeakSegDisk> provides an on-disk implementation of optimal log-linear algorithms for computing multiple peaks in a single sample. Computes same models as PeakSegOptimal but works for much larger data sets because disk is used for storage instead of memory. Citation: JSS'22, <https://www.jstatsoft.org/article/view/v101i10>

PeakSegJoint <https://CRAN.R-project.org/package=PeakSegJoint> provides a fast heuristic algorithm for computing models with a single common peak in $0, \dots, S$ samples. Citation: PSB'20 <http://psb.stanford.edu/psb-online/proceedings/psb20/Hocking.pdf>

PeakSegPipeline <https://github.com/tdhock/PeakSegPipeline> provides a pipeline for genome-wide peak calling using the other PeakSeg packages.

The remainder of this vignette is dedicated to an explanation of how to use PeakSegDisk.

2 Simulate a noisy integer vector with changes

The first example we will treat is detecting peaks in a vector of integer data, with possibly the same values at adjacent positions. This is an inefficient representation for large genomic data, but it is the typical output from simulation functions like `rpois`:

```
sim.seg <- function(seg.mean, size.mean=15){
  seg.size <- rpois(1, size.mean)
  rpois(seg.size, seg.mean)
}
set.seed(1)
seg.mean.vec <- c(1.5, 3.5, 0.5, 4.5, 2.5)
z.list <- lapply(seg.mean.vec, sim.seg)
(z.rep.vec <- unlist(z.list))

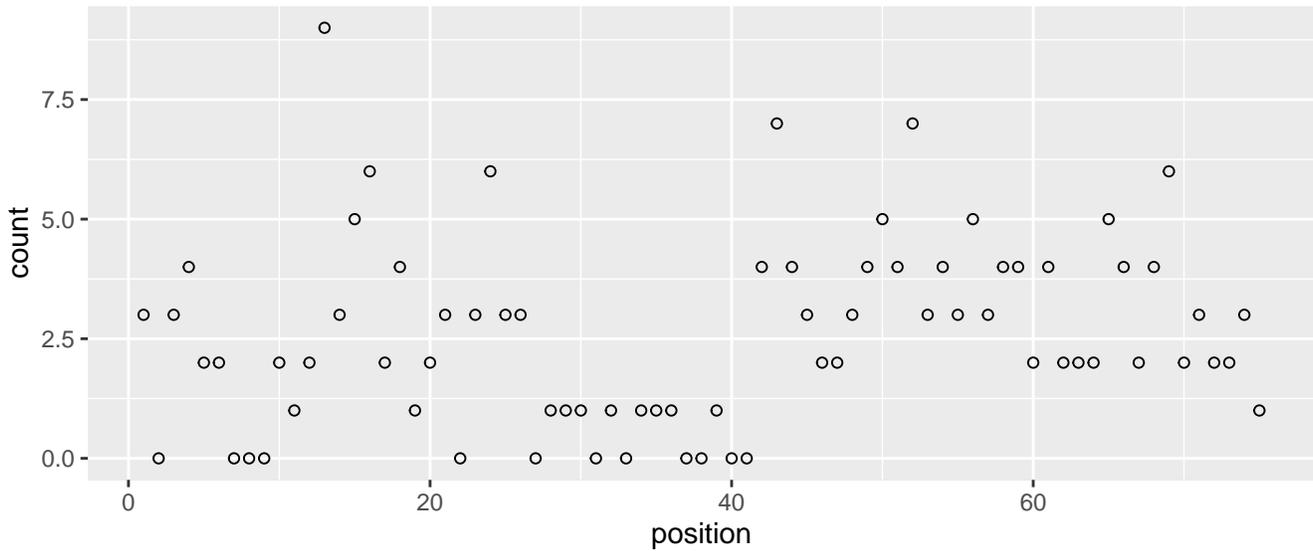
#> [1] 3 0 3 4 2 2 0 0 0 2 1 2 9 3 5 6 2 4 1 2 3 0 3 6 3 3 0 1 1 1 0 1 0 1 1 1 0 0
#> [39] 1 0 0 4 7 4 3 2 2 3 4 5 4 7 3 4 3 5 3 4 4 2 4 2 2 2 5 4 2 4 6 2 3 2 2 3 1
```

From the output above it is clear that these simulated data are integers, with some identical values at adjacent positions.

Below we put these data into a data table in order to plot them along with the model using `ggplot2`:

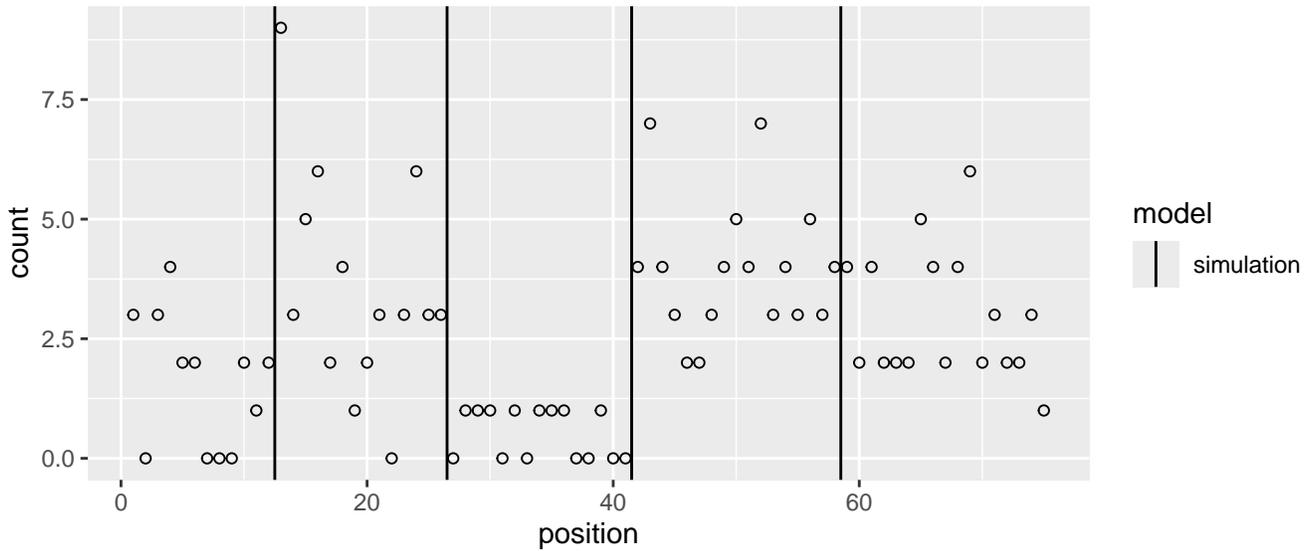
```
count.df <- data.frame(
  chrom="chrUnknown",
  chromStart=0:(length(z.rep.vec)-1),
  chromEnd=1:length(z.rep.vec),
  count=z.rep.vec)
if(require(ggplot2)){
  gg.count <- ggplot()+
    xlab("position")+
    geom_point(aes(
      chromEnd, count),
      shape=1,
      data=count.df)
  gg.count
}

#> Loading required package: ggplot2
```



The true changepoints in the simulation are shown below.

```
n.segs <- length(seg.mean.vec)
seg.size.vec <- sapply(z.list, length)
seg.end.vec <- cumsum(seg.size.vec)
change.vec <- seg.end.vec[-n.segs]+0.5
change.df <- data.frame(
  changepoint=change.vec)
if(require(ggplot2)){
gg.change <- gg.count+
  geom_vline(aes(
    xintercept=changepoint, color=model),
    data=data.frame(change.df, model="simulation"))+
  scale_color_manual(
    values=c(
      simulation="black",
      fitted="green"))
gg.change
}
```



3 Segment a vector of integers

Let $z_1, \dots, z_n \in \mathbb{Z}_+$ be the sequence of n non-negative count data in `z.rep.vec`, and let $w_1 = \dots = w_n = 1$ be weights which are all 1. The peak detection algorithm computes the solution to the following optimization problem:

$$\begin{aligned} & \underset{\substack{\mathbf{m} \in \mathbb{R}^n, \mathbf{s} \in \{0,1\}^n \\ \mathbf{c} \in \{-1,0,1\}^{n-1}}}{\text{minimize}} && \sum_{i=1}^n w_i \ell(m_i, z_i) + \lambda \sum_{i=1}^{n-1} I(c_i = 1) \\ & \text{subject to} && \text{no change: } c_i = 0 \Rightarrow m_i = m_{i+1} \text{ and } s_i = s_{i+1} \\ & && \text{go up: } c_i = 1 \Rightarrow m_i \leq m_{i+1} \text{ and } (s_i, s_{i+1}) = (0, 1), \\ & && \text{go down: } c_i = -1 \Rightarrow m_i \geq m_{i+1} \text{ and } (s_i, s_{i+1}) = (1, 0), \\ & && \text{start and end down: } s_1 = s_n = 0. \end{aligned}$$

where $\ell(m, z) = m - z \log m$ is the Poisson loss. The optimization variables are m_i for the segment mean, s_i for hidden state, and c_i for type of changepoint. The penalty term is proportional to the number of changepoint variables c_i which are equal to 1 (which is the same as the number of peaks in the resulting model).

To run the peak detection algorithm a numeric penalty parameter $\lambda \geq 0$ must be specified by the user. The smallest value is 0 which yields max peaks, and the largest value is Inf which yields no peaks. The code below runs the peak detection algorithm on this count data vector, using the penalty parameter $\lambda = 10.5$:

```
fit <- list()
(fit$vec <- PeakSegDisk::PeakSegFPOP_vec(z.rep.vec, 10.5))

#> $segments
#>      chrom chromStart chromEnd      status      mean
#>      <char>      <int>      <int>      <char>      <num>
```

```

#> 1: chrUnknown      69      75 background 2.166670
#> 2: chrUnknown      41      69      peak 3.714290
#> 3: chrUnknown      26      41 background 0.533333
#> 4: chrUnknown      12      26      peak 3.571430
#> 5: chrUnknown       0      12 background 1.583330
#>
#> $loss
#>   penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>   <num>   <int> <int> <int>           <int>           <num>       <num>
#> 1:   10.5     5    2   75             60    0.01507491 -19.86938
#>   equality.constraints mean.intervals max.intervals  megabytes seconds
#>           <int>           <num>           <int>       <num>  <num>
#> 1:                0             4.6             8 0.01372147  0.006
#>
#> $data
#>   chrom chromStart chromEnd count
#>   <char>   <int>   <int> <int>
#> 1: chrUnknown     0     1    3
#> 2: chrUnknown     1     2    0
#> 3: chrUnknown     2     3    3
#> 4: chrUnknown     3     4    4
#> 5: chrUnknown     4     6    2
#> 6: chrUnknown     6     9    0
#> 7: chrUnknown     9    10    2
#> 8: chrUnknown    10    11    1
#> 9: chrUnknown    11    12    2
#> 10: chrUnknown   12    13    9
#> 11: chrUnknown   13    14    3
#> 12: chrUnknown   14    15    5
#> 13: chrUnknown   15    16    6
#> 14: chrUnknown   16    17    2
#> 15: chrUnknown   17    18    4
#> 16: chrUnknown   18    19    1
#> 17: chrUnknown   19    20    2
#> 18: chrUnknown   20    21    3
#> 19: chrUnknown   21    22    0
#> 20: chrUnknown   22    23    3
#> 21: chrUnknown   23    24    6
#> 22: chrUnknown   24    26    3
#> 23: chrUnknown   26    27    0
#> 24: chrUnknown   27    30    1
#> 25: chrUnknown   30    31    0
#> 26: chrUnknown   31    32    1
#> 27: chrUnknown   32    33    0
#> 28: chrUnknown   33    36    1
#> 29: chrUnknown   36    38    0

```

```

#> 30: chrUnknown      38      39      1
#> 31: chrUnknown      39      41      0
#> 32: chrUnknown      41      42      4
#> 33: chrUnknown      42      43      7
#> 34: chrUnknown      43      44      4
#> 35: chrUnknown      44      45      3
#> 36: chrUnknown      45      47      2
#> 37: chrUnknown      47      48      3
#> 38: chrUnknown      48      49      4
#> 39: chrUnknown      49      50      5
#> 40: chrUnknown      50      51      4
#> 41: chrUnknown      51      52      7
#> 42: chrUnknown      52      53      3
#> 43: chrUnknown      53      54      4
#> 44: chrUnknown      54      55      3
#> 45: chrUnknown      55      56      5
#> 46: chrUnknown      56      57      3
#> 47: chrUnknown      57      59      4
#> 48: chrUnknown      59      60      2
#> 49: chrUnknown      60      61      4
#> 50: chrUnknown      61      64      2
#> 51: chrUnknown      64      65      5
#> 52: chrUnknown      65      66      4
#> 53: chrUnknown      66      67      2
#> 54: chrUnknown      67      68      4
#> 55: chrUnknown      68      69      6
#> 56: chrUnknown      69      70      2
#> 57: chrUnknown      70      71      3
#> 58: chrUnknown      71      73      2
#> 59: chrUnknown      73      74      3
#> 60: chrUnknown      74      75      1
#>      chrom chromStart chromEnd count
#>      <char>      <int>      <int> <int>
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_df" "PeakSegFPOP_dir" "list"

```

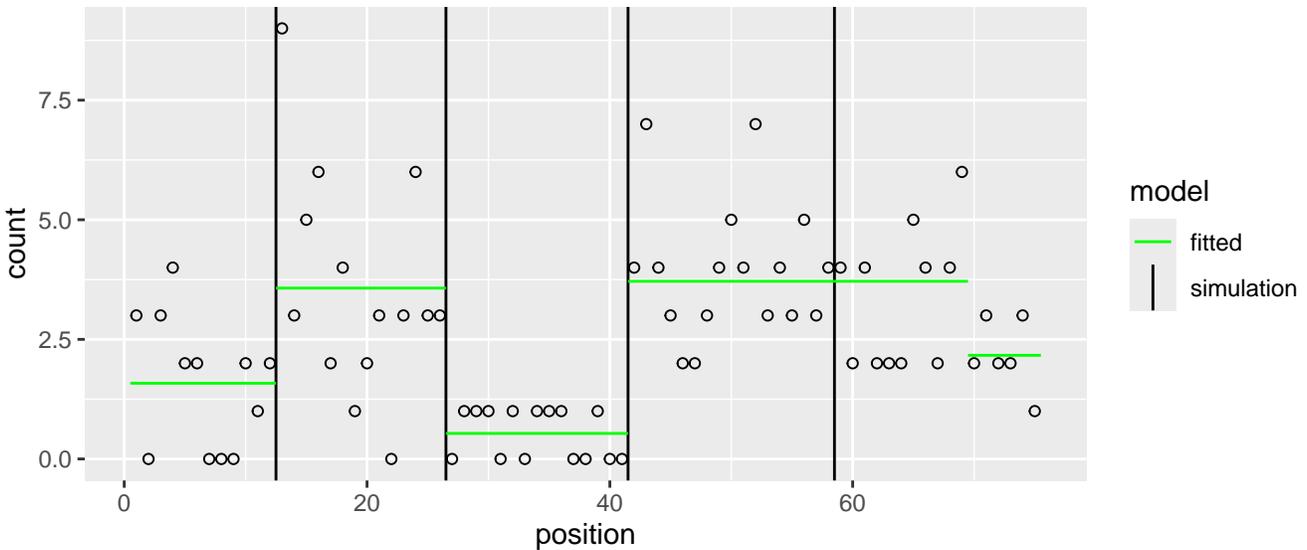
The model output list above includes `segments`, a data table with one row for each segment mean, and `loss`, a data table with one row that reports the model meta-data. Of interest are:

- `penalty`, the user-provided penalty value,
- `segments`, the number of segments,
- `peaks`, the number of peaks (even-numbered segments),
- `bases`, the number of data points in repetitive form (not run-length encoding),

- `bedGraph.lines`, the number of data points in run-length encoding form,
- `mean.pen.cost`, the optimal mean loss plus $\text{penalty} \times \text{peaks}$,
- `total.loss`, the optimal total Poisson loss over all data points,
- `equality.constraints`, the number of adjacent segment means that are equal in the optimal solution. Note that when this number is greater than 0, then there are some active equality constraints, and the optimal model is therefore not feasible for the strict inequality constraints, which implies that the optimum of the problem with strict inequality constraints is undefined, i.e. for any sub-optimal solution that satisfies the strict inequality constraints, we can find a lower cost solution that satisfies the strict inequality constraints (but is still sub-optimal), by getting closer to the solution with active equality constraints.
- `megabytes`, the storage space on disk used by the solver,
- `seconds`, the amount of time used by the solver,
- `mean.intervals`, `max.intervals`, statistics over all intervals (candidate changepoints) computed by the functional pruning algorithm, useful for analyzing computational complexity, which is linear in the number of intervals.

Note in particular that `PeakSegFPOP_vec` internally uses `rle` to construct a run-length encoding, which is passed to the solver to save time/storage. In this case the repetitive integer data vector contains 75 elements but the `coverage.bedGraph` data file contains only 60 lines. In real genomic data sets the difference is typically much larger.

```
gg.change+
  geom_segment(aes(
    chromStart+0.5, mean, xend=chromEnd+0.5, yend=mean, color=model),
    data=data.frame(fit$vec$segments, model="fitted"))
```

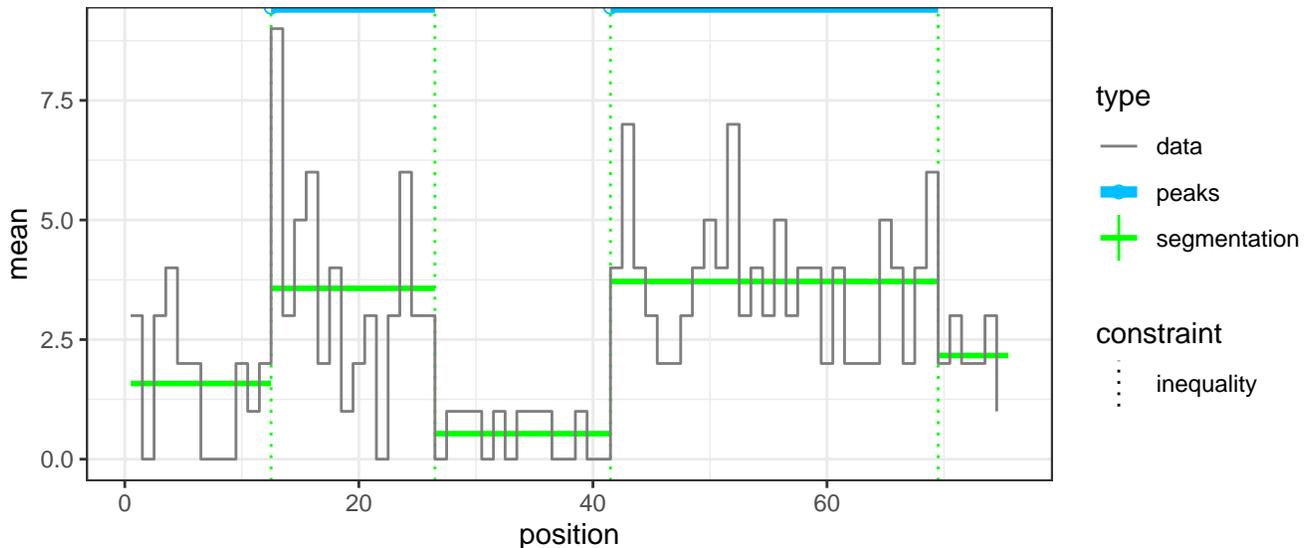


It is clear from the plot above that the first three changepoints are estimated exactly and the last one is a bit over-estimated.

Also note that a default plot method is defined for these objects:

```
plot(fit$vec)
```

```
#> Warning: Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.  
#> i Please use 'linewidth' instead.  
#> i The deprecated feature was likely used in the PeakSegDisk package.  
#> Please report the issue at <https://github.com/tdhock/PeakSegDisk/issues>.  
#> This warning is displayed once per session.  
#> Call 'lifecycle::last_lifecycle_warnings()' to see where this warning was  
#> generated.
```



4 Segment a data frame

Another interface that can be used on a data.frame with n rows and exactly 4 columns (chrom, chromStart, chromEnd, count) is `PeakSegFPOP_df`. For each row $i \in \{1, \dots, n\}$, let $z_i \in \mathbb{Z}_+$ be the non-negative count data (count column), and let $w_i > 0$ be the weight (equal to the number of bases, $\text{chromEnd} - \text{chromStart}$). The optimization problem we solve is the same as before. Note that this function does not perform run-length encoding for you:

```
(fit$df <- PeakSegDisk::PeakSegFPOP_df(count.df, 10.5))
```

```
#> $segments  
#>      chrom chromStart chromEnd  status  mean  
#>      <char>      <int>   <int>   <char> <num>  
#> 1: chrUnknown      69     75 background 2.166670  
#> 2: chrUnknown      41     69      peak 3.714290  
#> 3: chrUnknown      26     41 background 0.533333  
#> 4: chrUnknown      12     26      peak 3.571430  
#> 5: chrUnknown       0     12 background 1.583330  
#>  
#> $loss
```

```

#>   penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>   <num>   <int> <int> <int>           <int>           <num>       <num>
#> 1:   10.5     5    2   75             75    0.01507491 -19.86938
#>   equality.constraints mean.intervals max.intervals megabytes seconds
#>           <int>           <num>           <int>       <num>   <num>
#> 1:                0           4.633333           8 0.01725006   0.002
#>
#> $data
#>       chrom chromStart chromEnd count
#>       <char>      <int>    <int> <int>
#> 1: chrUnknown      0         1     3
#> 2: chrUnknown      1         2     0
#> 3: chrUnknown      2         3     3
#> 4: chrUnknown      3         4     4
#> 5: chrUnknown      4         5     2
#> 6: chrUnknown      5         6     2
#> 7: chrUnknown      6         7     0
#> 8: chrUnknown      7         8     0
#> 9: chrUnknown      8         9     0
#> 10: chrUnknown     9        10     2
#> 11: chrUnknown    10        11     1
#> 12: chrUnknown    11        12     2
#> 13: chrUnknown    12        13     9
#> 14: chrUnknown    13        14     3
#> 15: chrUnknown    14        15     5
#> 16: chrUnknown    15        16     6
#> 17: chrUnknown    16        17     2
#> 18: chrUnknown    17        18     4
#> 19: chrUnknown    18        19     1
#> 20: chrUnknown    19        20     2
#> 21: chrUnknown    20        21     3
#> 22: chrUnknown    21        22     0
#> 23: chrUnknown    22        23     3
#> 24: chrUnknown    23        24     6
#> 25: chrUnknown    24        25     3
#> 26: chrUnknown    25        26     3
#> 27: chrUnknown    26        27     0
#> 28: chrUnknown    27        28     1
#> 29: chrUnknown    28        29     1
#> 30: chrUnknown    29        30     1
#> 31: chrUnknown    30        31     0
#> 32: chrUnknown    31        32     1
#> 33: chrUnknown    32        33     0
#> 34: chrUnknown    33        34     1
#> 35: chrUnknown    34        35     1
#> 36: chrUnknown    35        36     1

```

```

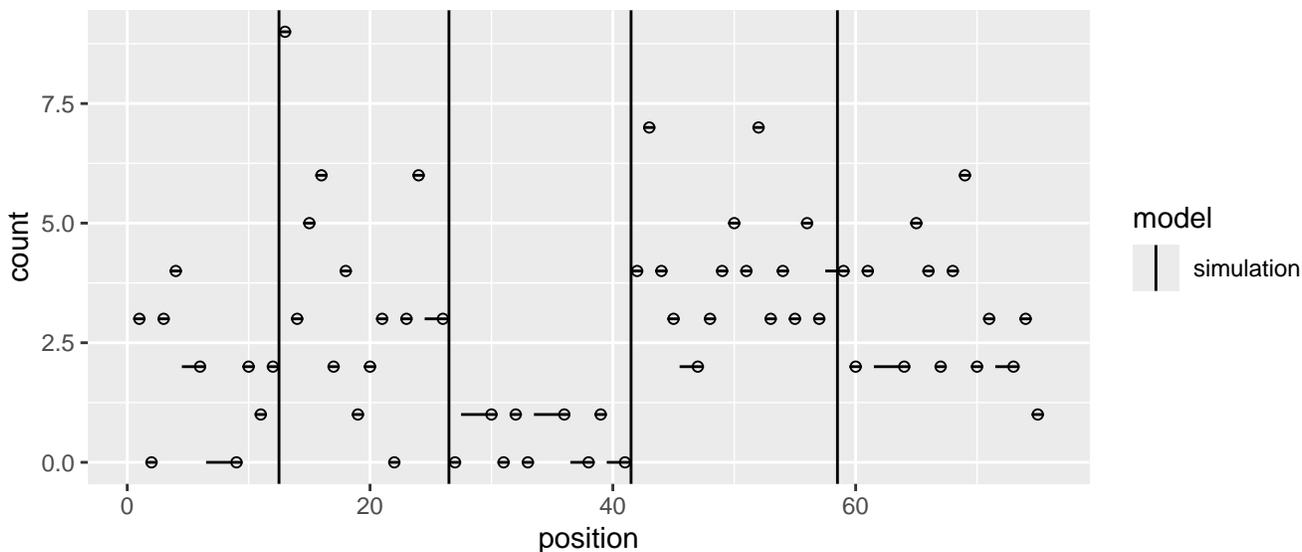
#> 37: chrUnknown      36      37      0
#> 38: chrUnknown      37      38      0
#> 39: chrUnknown      38      39      1
#> 40: chrUnknown      39      40      0
#> 41: chrUnknown      40      41      0
#> 42: chrUnknown      41      42      4
#> 43: chrUnknown      42      43      7
#> 44: chrUnknown      43      44      4
#> 45: chrUnknown      44      45      3
#> 46: chrUnknown      45      46      2
#> 47: chrUnknown      46      47      2
#> 48: chrUnknown      47      48      3
#> 49: chrUnknown      48      49      4
#> 50: chrUnknown      49      50      5
#> 51: chrUnknown      50      51      4
#> 52: chrUnknown      51      52      7
#> 53: chrUnknown      52      53      3
#> 54: chrUnknown      53      54      4
#> 55: chrUnknown      54      55      3
#> 56: chrUnknown      55      56      5
#> 57: chrUnknown      56      57      3
#> 58: chrUnknown      57      58      4
#> 59: chrUnknown      58      59      4
#> 60: chrUnknown      59      60      2
#> 61: chrUnknown      60      61      4
#> 62: chrUnknown      61      62      2
#> 63: chrUnknown      62      63      2
#> 64: chrUnknown      63      64      2
#> 65: chrUnknown      64      65      5
#> 66: chrUnknown      65      66      4
#> 67: chrUnknown      66      67      2
#> 68: chrUnknown      67      68      4
#> 69: chrUnknown      68      69      6
#> 70: chrUnknown      69      70      2
#> 71: chrUnknown      70      71      3
#> 72: chrUnknown      71      72      2
#> 73: chrUnknown      72      73      2
#> 74: chrUnknown      73      74      3
#> 75: chrUnknown      74      75      1
#>      chrom chromStart chromEnd count
#>      <char>      <int>      <int> <int>
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_df" "PeakSegFPOP_dir" "list"

```

Note how `bedGraph.lines` is now the same size as `bases`, 75. The time/storage complexity is log-linear in the number of `bedGraph.lines`, so it is more efficient to use the run-length encoding. This

can be easily done in R:

```
z.rle.vec <- rle(z.rep.vec)
chromEnd <- cumsum(z.rle.vec$lengths)
rle.df <- data.frame(
  chrom="chrUnknown",
  chromStart=c(0L, chromEnd[-length(chromEnd)]),
  chromEnd,
  count=z.rle.vec$values)
if(require(ggplot2)){
gg.rle <- ggplot()+
  geom_segment(aes(
    chromStart+0.5, count, xend=chromEnd+0.5, yend=count),
    data=rle.df)+
  geom_point(aes(
    chromEnd, count),
    shape=1,
    data=rle.df)+
  geom_vline(aes(
    xintercept=changepoint, color=model),
    data=data.frame(change.df, model="simulation"))+
  scale_color_manual(
    values=c(
      simulation="black",
      fitted="green"))+
  xlab("position")
gg.rle
}
```



The plot above shows the run-length encoded data, with a `geom_point` for the last position in each run, and a `geom_segment` extending left to the first position. These data can be segmented as above:

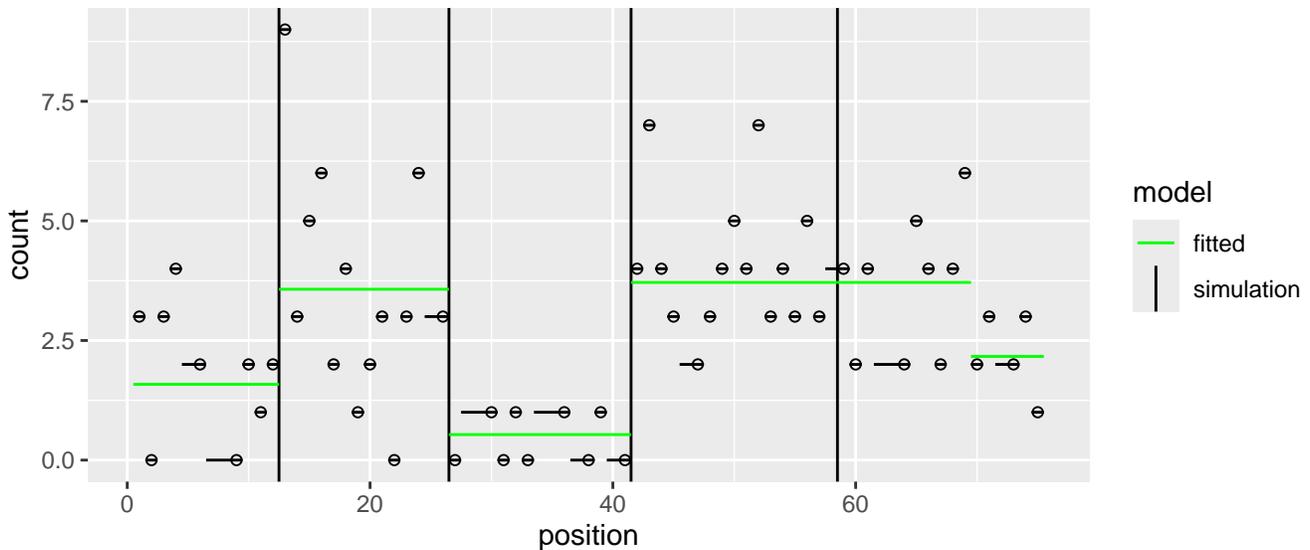
```
(fit$rle <- PeakSegDisk::PeakSegFPOP_df(rle.df, 10.5))

#> $segments
#>      chrom chromStart chromEnd      status      mean
#>      <char>      <int>   <int>   <char>   <num>
#> 1: chrUnknown      69      75 background 2.166670
#> 2: chrUnknown      41      69      peak 3.714290
#> 3: chrUnknown      26      41 background 0.533333
#> 4: chrUnknown      12      26      peak 3.571430
#> 5: chrUnknown       0      12 background 1.583330
#>
#> $loss
#>      penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>      <num>      <int> <int> <int>          <int>          <num>      <num>
#> 1:    10.5         5     2   75             60      0.01507491 -19.86938
#>      equality.constraints mean.intervals max.intervals megabytes seconds
#>      <int>          <num>          <int>          <num>      <num>
#> 1:              0            4.6              8 0.01372147  0.002
#>
#> $data
#>      chrom chromStart chromEnd count
#>      <char>      <int>   <int> <int>
#> 1: chrUnknown      0       1     3
#> 2: chrUnknown      1       2     0
#> 3: chrUnknown      2       3     3
#> 4: chrUnknown      3       4     4
#> 5: chrUnknown      4       6     2
#> 6: chrUnknown      6       9     0
#> 7: chrUnknown      9      10     2
#> 8: chrUnknown     10      11     1
#> 9: chrUnknown     11      12     2
#> 10: chrUnknown    12      13     9
#> 11: chrUnknown    13      14     3
#> 12: chrUnknown    14      15     5
#> 13: chrUnknown    15      16     6
#> 14: chrUnknown    16      17     2
#> 15: chrUnknown    17      18     4
#> 16: chrUnknown    18      19     1
#> 17: chrUnknown    19      20     2
#> 18: chrUnknown    20      21     3
#> 19: chrUnknown    21      22     0
#> 20: chrUnknown    22      23     3
#> 21: chrUnknown    23      24     6
#> 22: chrUnknown    24      26     3
#> 23: chrUnknown    26      27     0
#> 24: chrUnknown    27      30     1
#> 25: chrUnknown    30      31     0
```

```

#> 26: chrUnknown      31      32      1
#> 27: chrUnknown      32      33      0
#> 28: chrUnknown      33      36      1
#> 29: chrUnknown      36      38      0
#> 30: chrUnknown      38      39      1
#> 31: chrUnknown      39      41      0
#> 32: chrUnknown      41      42      4
#> 33: chrUnknown      42      43      7
#> 34: chrUnknown      43      44      4
#> 35: chrUnknown      44      45      3
#> 36: chrUnknown      45      47      2
#> 37: chrUnknown      47      48      3
#> 38: chrUnknown      48      49      4
#> 39: chrUnknown      49      50      5
#> 40: chrUnknown      50      51      4
#> 41: chrUnknown      51      52      7
#> 42: chrUnknown      52      53      3
#> 43: chrUnknown      53      54      4
#> 44: chrUnknown      54      55      3
#> 45: chrUnknown      55      56      5
#> 46: chrUnknown      56      57      3
#> 47: chrUnknown      57      59      4
#> 48: chrUnknown      59      60      2
#> 49: chrUnknown      60      61      4
#> 50: chrUnknown      61      64      2
#> 51: chrUnknown      64      65      5
#> 52: chrUnknown      65      66      4
#> 53: chrUnknown      66      67      2
#> 54: chrUnknown      67      68      4
#> 55: chrUnknown      68      69      6
#> 56: chrUnknown      69      70      2
#> 57: chrUnknown      70      71      3
#> 58: chrUnknown      71      73      2
#> 59: chrUnknown      73      74      3
#> 60: chrUnknown      74      75      1
#>      chrom chromStart chromEnd count
#>      <char>      <int>      <int> <int>
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_df" "PeakSegFPOP_dir" "list"
if(require(ggplot2)){
gg.rle+
  geom_segment(aes(
    chromStart+0.5, mean, xend=chromEnd+0.5, yend=mean, color=model),
    data=data.frame(fit$rle$segments, model="fitted"))
}

```



5 Write the file yourself

The interfaces discussed in the previous sections are perhaps the most intuitive for useRs, but they are also the least efficient, so they are not recommended for large data.

In this section we introduce the most efficient way of using PeakSegDisk, which involves:

- creating a “problem” directory for each segmentation problem (sample and genome subset),
- saving the data to `coverage.bedGraph` in that directory,
- and then running `PeakSegFPOP_dir`.

The reason why this method is recommended for large data is because `PeakSegFPOP_dir` saves its results to the “problem” directory. So if a certain result has already been computed, these result files are used as a cache, and are read instead of doing computations, which saves a lot of time. The file system is used as the interface in order to support very large data sets with very little memory usage.

To use `PeakSegFPOP_dir` the data should be saved to a `chrXX-start-end/coverage.bedGraph` file, where the problem directory “chrXX-start-end” should be named using a genome position string:

- chrXX is the chromosome (which is irrelevant to the algorithm),
- start is the 0-based first position of the region to segment (the smallest possible value is 0),
- end is the 1-based end position (the smallest possible value is 1).

```
data.dir <- file.path(
  tempfile(),
  with(rle.df, sprintf(
    "%s-%d-%d", chrom[1], min(chromStart), max(chromEnd))))
```

```
dir.create(data.dir, showWarnings=FALSE, recursive=TRUE)
coverage.bedGraph <- file.path(data.dir, "coverage.bedGraph")
write.table(
  rle.df, coverage.bedGraph,
  sep="\t", row.names=FALSE, col.names=FALSE)
```

The next step is to run the main solver,

```
(fit$dir <- PeakSegDisk::PeakSegFPOP_dir(data.dir, 10.5))

#> $segments
#>      chrom chromStart chromEnd      status      mean
#>      <char>      <int>      <int>      <char>      <num>
#> 1: chrUnknown      69        75 background 2.166670
#> 2: chrUnknown      41        69      peak 3.714290
#> 3: chrUnknown      26        41 background 0.533333
#> 4: chrUnknown      12        26      peak 3.571430
#> 5: chrUnknown       0        12 background 1.583330
#>
#> $loss
#>  penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>      <num>      <int> <int> <int>      <int>      <num>      <num>
#> 1:    10.5         5     2    75          60    0.01507491 -19.86938
#>  equality.constraints mean.intervals max.intervals  megabytes seconds
#>      <int>      <num>      <int>      <num>      <num>
#> 1:          0         4.6          8 0.01372147  0.002
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_dir" "list"
```

The underlying C++ code creates penalty-specific files such as

`chrXX-start-end/coverage.bedGraph_penalty=0.1_loss.tsv` which are used to store/cache the results. If the files already exist (and are consistent) then `PeakSegFPOP_dir` just reads them; otherwise it runs the dynamic programming C++ code in order to create those files, which are then read into R.

6 Computing the model with a given number of peaks

The `sequentialSearch_dir` function can be used to compute the optimal model with a certain number of peaks:

```
if(interactive() && requireNamespace("future"))future::plan("multisession")
(fit$search <- PeakSegDisk::sequentialSearch_dir(data.dir, 2L, verbose=1))

#> Loading required namespace: future.apply
```

```

#> Next = 0, Inf
#> Next = 2.20991803112367
#> Next = 7.11950550040458
#> $segments
#>      chrom chromStart chromEnd      status      mean
#>      <char>      <int>      <int>      <char>      <num>
#> 1: chrUnknown      69         75 background 2.166670
#> 2: chrUnknown      41         69         peak 3.714290
#> 3: chrUnknown      26         41 background 0.533333
#> 4: chrUnknown      12         26         peak 3.571430
#> 5: chrUnknown       0         12 background 1.583330
#>
#> $loss
#>      penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>      <num>      <int> <int> <int>      <int>      <num>      <num>
#> 1: 7.119506         5      2      75          60 -0.07507161 -19.86938
#>      equality.constraints mean.intervals max.intervals megabytes seconds
#>      <int>      <num>      <int>      <num>      <num>
#> 1:              0          4.558333          9 0.0136261  0.002
#>      iteration under over
#>      <num> <int> <int>
#> 1:         3      0      6
#>
#> $others
#>      penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#>      <num>      <int> <int> <int>      <int>      <num>      <num>
#> 1: 0.000000         53      26      75          60 -0.63772877 -47.829658
#> 2:      Inf          1       0      75          60  0.12837615  9.628211
#> 3: 2.209918         13       6      75          60 -0.26439085 -33.088822
#> 4: 7.119506          5       2      75          60 -0.07507161 -19.869382
#>      equality.constraints mean.intervals max.intervals  megabytes seconds
#>      <int>      <num>      <int>      <num>      <num>
#> 1:              5          2.550000          4 0.009029388  0.002
#> 2:              0          0.000000          0 0.000000000  0.001
#> 3:              0          4.708333          9 0.013969421  0.002
#> 4:              0          4.558333          9 0.013626099  0.002
#>      iteration under over
#>      <num> <int> <int>
#> 1:         1     NA     NA
#> 2:         1     NA     NA
#> 3:         2       0     26
#> 4:         3       0      6
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_dir" "list"

```

The algorithm must evaluate several penalty values to compute the optimal model with a certain

number of peaks. The `others` component of the model list above shows that

- the search starts with penalty values 0 and Inf, which result in models with 26 and 0 peaks, respectively.
- the next penalty evaluated is 2.21, which results in 6 peaks.
- the final penalty evaluated is 7.12, which results in 2 peaks.

At each step (except the first) the new penalties are computed based on the loss values found in the previous step. If present with a registered parallel future plan, the `future.apply` package is used to run the first step (penalties 0, ∞) in parallel.

Note how the number of peaks and `total.loss` of this model is the same as the other models computed above,

```
lossDF <- function(L)data.frame(L$loss)[, names(fit$dir$loss)]
do.call(rbind, lapply(fit, lossDF))

#>      penalty segments peaks bases bedGraph.lines mean.pen.cost total.loss
#> vec    10.500000      5     2    75           60  0.01507491 -19.86938
#> df     10.500000      5     2    75           75  0.01507491 -19.86938
#> rle    10.500000      5     2    75           60  0.01507491 -19.86938
#> dir    10.500000      5     2    75           60  0.01507491 -19.86938
#> search  7.119506      5     2    75           60 -0.07507161 -19.86938
#>      equality.constraints mean.intervals max.intervals  megabytes seconds
#> vec                0      4.600000      8 0.01372147  0.006
#> df                  0      4.633333      8 0.01725006  0.002
#> rle                  0      4.600000      8 0.01372147  0.002
#> dir                  0      4.600000      8 0.01372147  0.002
#> search                0      4.558333      9 0.01362610  0.002
```

Finally we demonstrate how the filesystem caching is especially useful for the sequential search. In the code below we ask the sequential search algorithm to compute the optimal model with four peaks:

```
four.peaks <- PeakSegDisk::sequentialSearch_dir(data.dir, 4L)
four.peaks$others[, .(iteration, penalty, peaks)]

#>   iteration  penalty peaks
#>      <num>    <num> <int>
#> 1:         1 0.000000    26
#> 2:         1      Inf     0
#> 3:         2 2.209918     6
#> 4:         3 7.119506     2
#> 5:         4 3.304860     3
#> 6:         5 2.830674     5
#> 7:         6 3.107790     4
```

Looking at the output above, we see that the first three iterations of the sequential search require computing models with 26, 0, 6, 2 peaks. Since all of these have been previously computed (and saved

to disk), the dynamic programming algorithm does not need to be re-run, and instead the model results are simply read from the files. After that the dynamic programming is run for the subsequent iterations 4-6. In this particular example the savings in computation time is not extraordinary, but in real genomic data, this can result in substantial speed-ups.