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 $0, ..., S$ 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

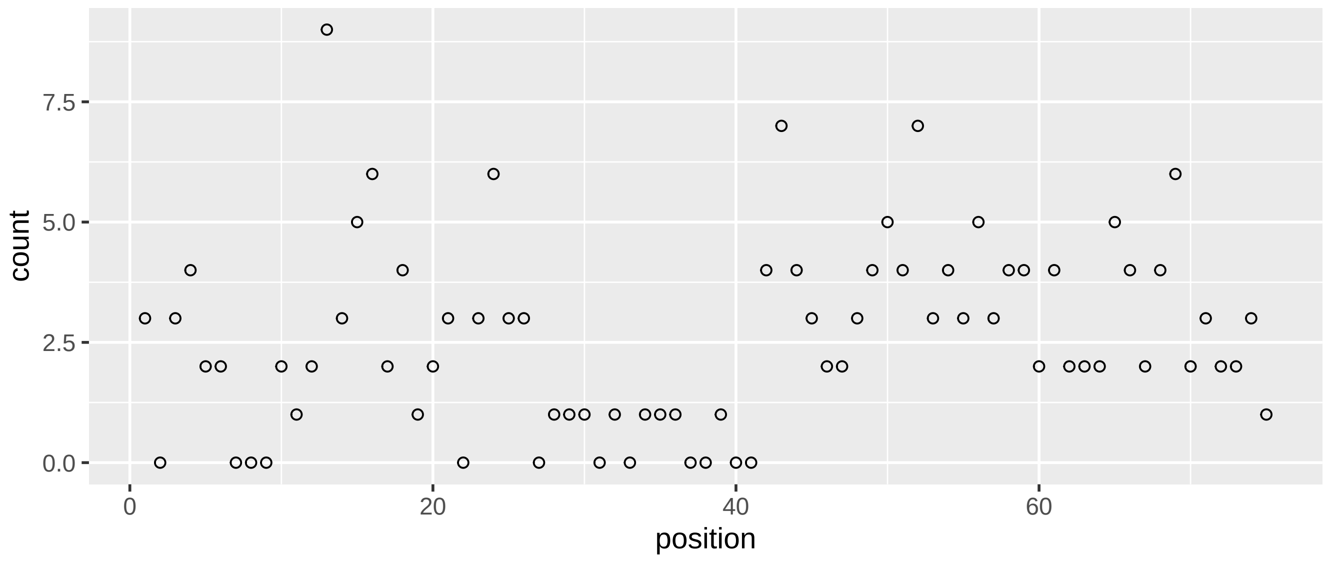
The first example we will treat is detecting peaks in a vector of integer data, with possibly the same values at adjacent positions. This is an inefficient representation for large genomic data, but it is the typical output from simulation functions like `rpois`:

```
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.

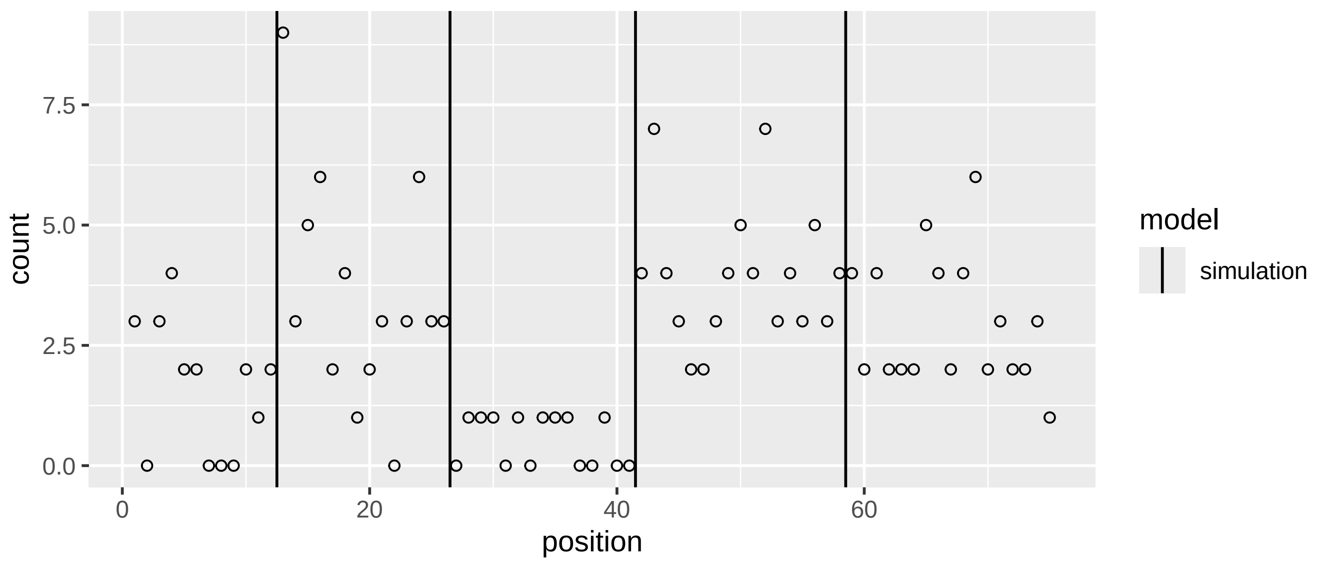
Below we put these data into a data table in order to plot them along with the model using ggplot2:

```
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
}

#> Le chargement a nécessité le 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 $w_1 = \cdots = w_n = 1$ be weights which are all 1. The peak detection algorithm computes the solution to the following optimization problem:

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

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   0.018
#>
#> $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
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_df"  "PeakSegFPOP_dir" "list"
```

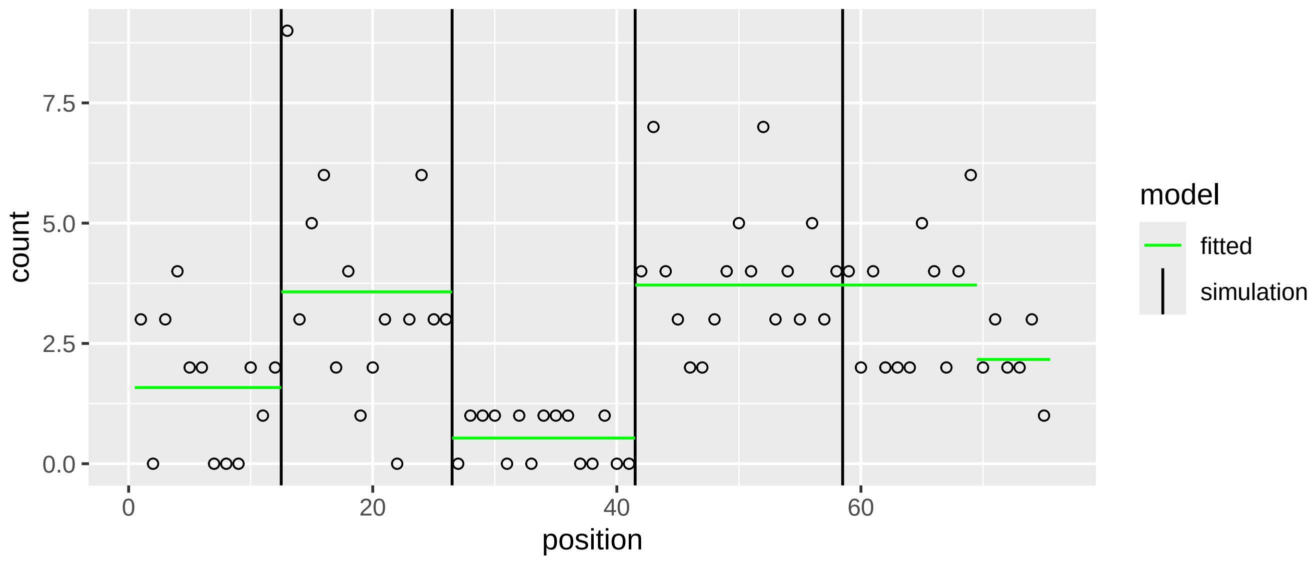
The model output list above includes `segments`, a data table with one row for each segment mean, and `loss`, a data table with one row that reports the model meta-data. Of interest are:

- `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 penalty*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 satifies 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.

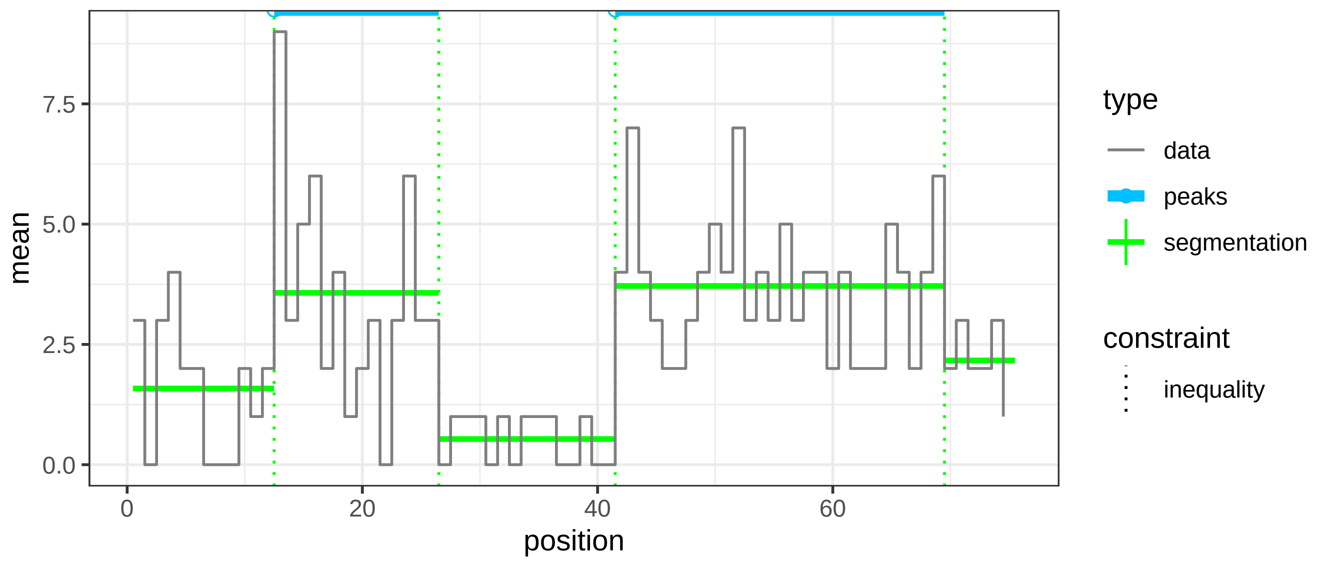
```
gg.change+
  geom_segment(aes(
    chromStart+0.5, mean, xend=chromEnd+0.5, yend=mean, color=model),
    data=data.frame(fit$vec$segments, model="fitted"))
```



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:

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



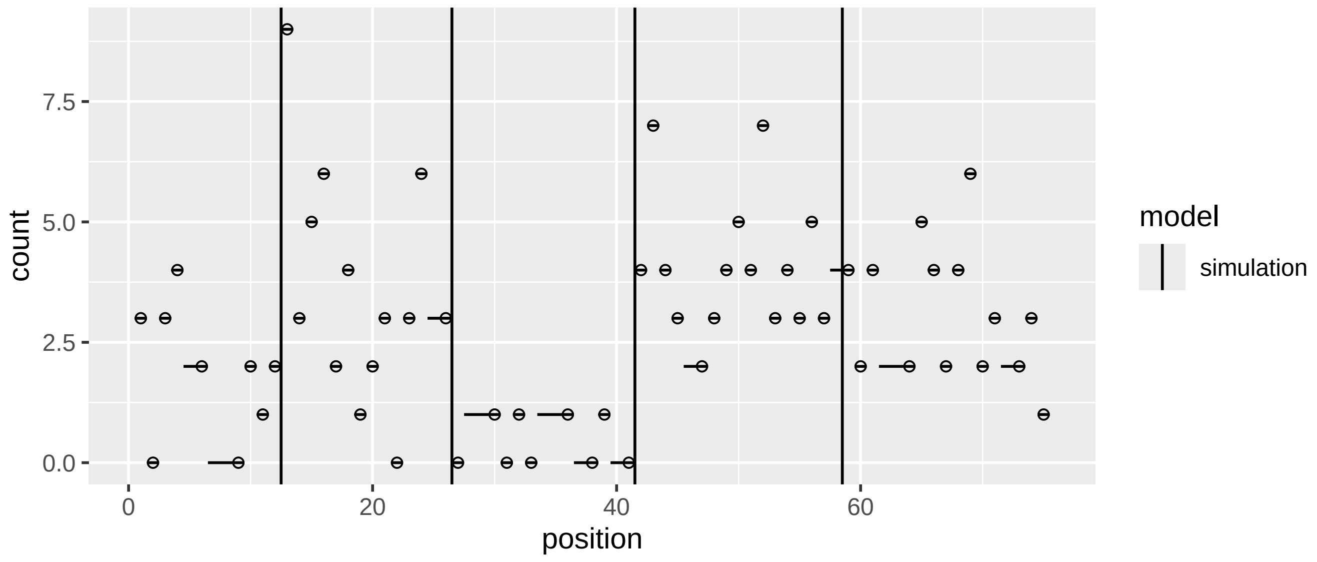
4 Segment a data frame

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, chromEnd-chromStart). The optimization problem we solve is the same as before. Note that this function does not perform run-length encoding for you:

```r
(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    0.01
#>
#> $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
#>
#> attr(,"class")
#> [1] "PeakSegFPOP_df"  "PeakSegFPOP_dir" "list"
```

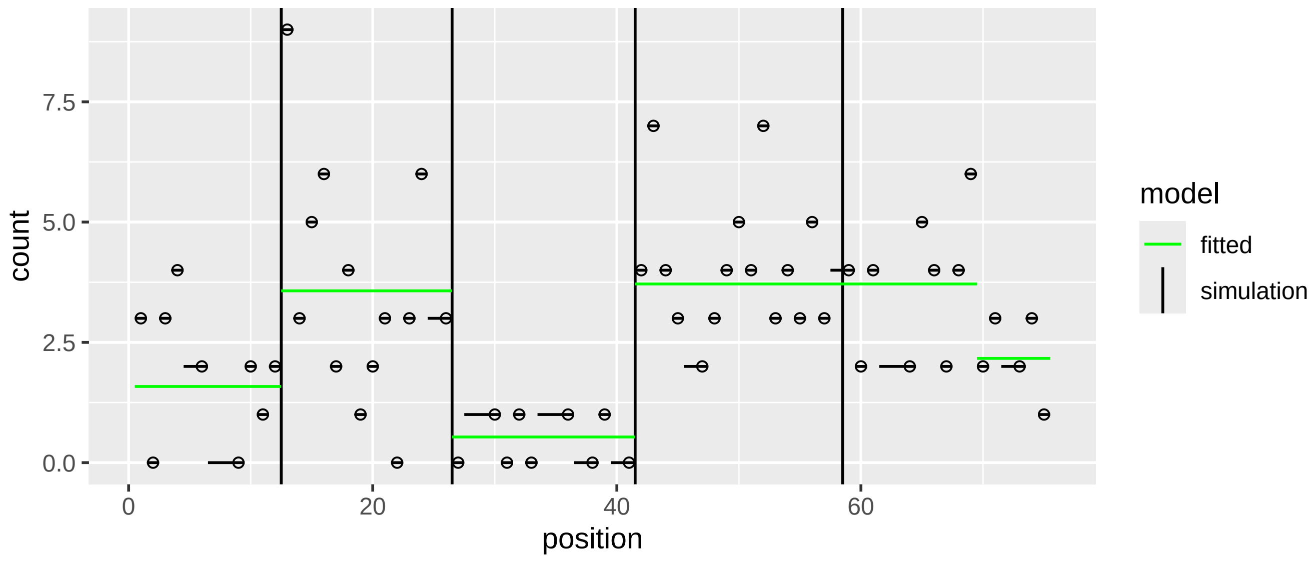
Note how `bedGraph.lines` is now the same size as `bases`, 75. The time/storage complexity is log-linear in the number of `bedGraph.lines`, so it is more efficient to use the run-length encoding. This can be easily done in R:

```
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   0.004
#>
#> $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
#>
#> 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 postion 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    0.01
#>
#> 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))

#> Le chargement a nécessité le package :  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   0.004
#>    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   0.013
#> 2:                    0       0.000000             0 0.000000000   0.001
#> 3:                    0       4.708333             9 0.013969421   0.013
#> 4:                    0       4.558333             9 0.013626099   0.004
#>    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 $0, \infty$) 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   0.018
#> df                        0       4.633333             8 0.01725006   0.010
#> rle                       0       4.600000             8 0.01372147   0.004
#> dir                       0       4.600000             8 0.01372147   0.010
#> search                    0       4.558333             9 0.01362610   0.004
```

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)

#> Le chargement a nécessité le package :  future.apply

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.