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, 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, but it is neither fast nor optimal, so in practice we recommend to use our newer packages below instead.

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.

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.

PeakSegJoint provides a fast heuristic algorithm for computing models with a single common peak in 0,...,S samples.

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
#> [36]  1  0  0  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
#> [71]  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)
library(ggplot2)
gg.count <- ggplot()+
    xlab("position")+
    geom_point(aes(
        chromEnd, count),
        shape=1,
        data=count.df)
gg.count

The true changepoints in the simulation are shown below.
3 Segment a vector of integers

Let \( z_1, \ldots, z_n \in \mathbb{Z}_+ \) be the sequence of non-negative count data in \( z.\text{rep.vec} \), 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:

\[
\text{minimize} \quad \sum_{i=1}^{n} w_i \ell(m_i, z_i) + \lambda \sum_{i=1}^{n-1} I(c_i = 1)
\]

subject to

- no change: \( c_i = 0 \Rightarrow m_i = m_{i+1} \) and \( s_i = s_{i+1} \)
- go up: \( c_i = 1 \Rightarrow m_i \leq m_{i+1} \) and \( (s_i, s_{i+1}) = (0, 1) \),
- go down: \( c_i = -1 \Rightarrow m_i \geq m_{i+1} \) and \( (s_i, s_{i+1}) = (1, 0) \),
- start and end down: \( s_1 = s_n = 0 \).
where \( f(m, z) = m - z \log m \) 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 \( \text{Inf} \) which yields no peaks. The code below runs the peak detection algorithm on this count data vector, using the penalty parameter \( \lambda = 10.5 \):

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

```r
#> $segments
#>      chrom chromStart chromEnd status    mean
#> 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
equality.constraints mean.intervals max.intervals megabytes seconds
#> 1:        10.5       5       2      75         60  0.01507491 -19.86938

#> $data
#>      chrom chromStart chromEnd count
#> 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

4
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 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.

```r
gg.change+
gem_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 \( i \in \{1, \ldots, n\} \), 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:
```
(fit$df <- PeakSegDisk::PeakSegFPOP_df(count.df, 10.5))

```$segments

<table>
<thead>
<tr>
<th>chrom</th>
<th>chromStart</th>
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<th>status</th>
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<tbody>
<tr>
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<td>69</td>
<td>75</td>
<td>background</td>
<td>2.1667</td>
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<td>background</td>
<td>1.5833</td>
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```$loss

<table>
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<th>bases</th>
<th>bedGraph.lines</th>
<th>mean.pen.cost</th>
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```$data

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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:

```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)

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:

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

```r
#> $segments
#>   chrom chromStart chromEnd status  mean
#> 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
#> 1:    10.5      5      2     75        60 0.01507491       -19.86938
#>
#> equality.constraints mean.intervals max.intervals megabytes seconds
#> 1:            0        4.6           8 0.01372147      0.01
#>
#> $data
#>   chrom chromStart chromEnd count
#> 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
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# 23: chrUnknown 26 27 0
# 24: chrUnknown 27 30 1
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# 26: chrUnknown 31 32 1
# 27: chrUnknown 32 33 0
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# 54: chrUnknown 67 68 4
# 55: chrUnknown 68 69 6
# 56: chrUnknown 69 70 2
# 57: chrUnknown 70 71 3
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).

```r
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
#> 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
#> 1: 10.5      5 2 75           60 0.01507491 -19.86938

#> 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:
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,

```r
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
#> vec 10.500000 5 2 75 60 0.01507491
#> df 10.500000 5 2 75 75 0.01507491
#> rle 10.500000 5 2 75 60 0.01507491
#> dir 10.500000 5 2 75 60 0.01507491
#> search 7.119506 5 2 75 60 -0.07507161
#> total.loss equality.constraints mean.intervals max.intervals
#> vec -19.86938 0 4.600000 8
#> df -19.86938 0 4.633333 8
#> rle -19.86938 0 4.600000 8
#> dir -19.86938 0 4.600000 8
#> search -19.86938 0 4.558333 9
#> megabytes seconds
#> vec 0.01372147 0.02
#> df 0.01725006 0.02
#> rle 0.01372147 0.01
#> dir 0.01372147 0.02
#> search 0.01362610 0.00
```

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:

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

```
#> iteration penalty peaks
#> 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.