Benchmarking

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Benchmarking of the different functions in the bendDNA package

In this R Markdown file all the different functions included in the bendDNA package are benchmarked. This will be done by looking at every function individually, testing and timing the functions for different parameter values.

The testing is done x times (depending on which function) and summary statistics are given in a summary table. These are then plotted using violin plots comparing every different parameter value. The CRAN microbenchmark package is used for making both the summary table and plot.

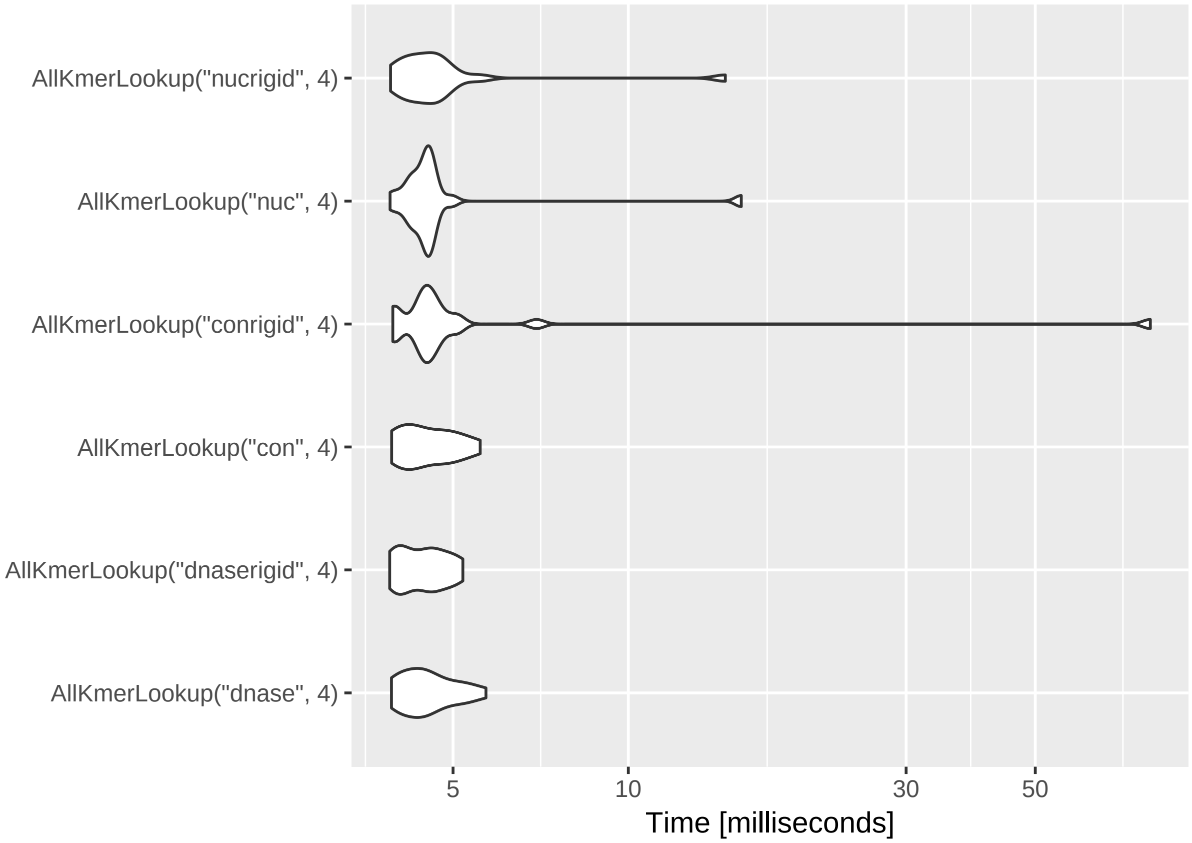
AllKmerLookup

Function for producing all possible k-mers and calculating their average bendability coefficients.

Usage: AllKmerLookup(scale, k, sequence.out = F)

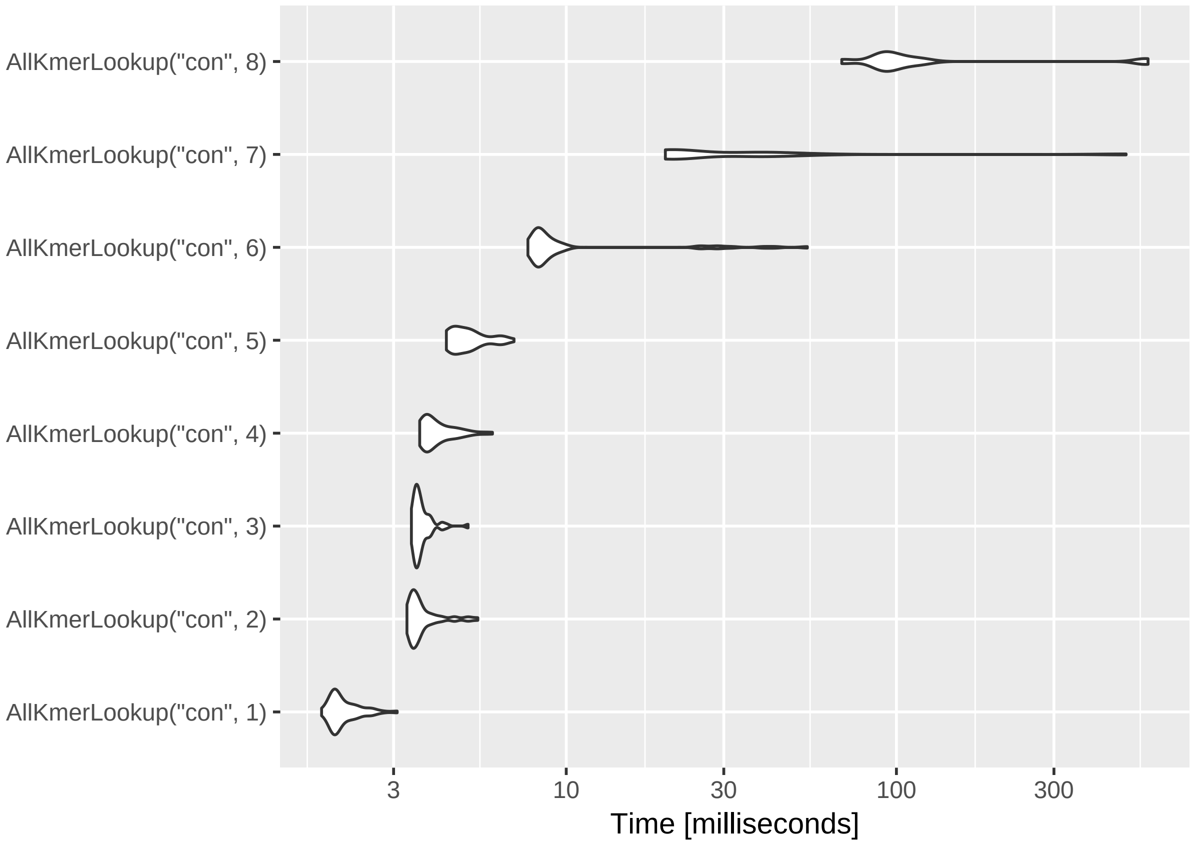
Parameters that can be used include: - Scale - Number of consecutive trinucleotides - Whether to output the sequences

Different lookup tables



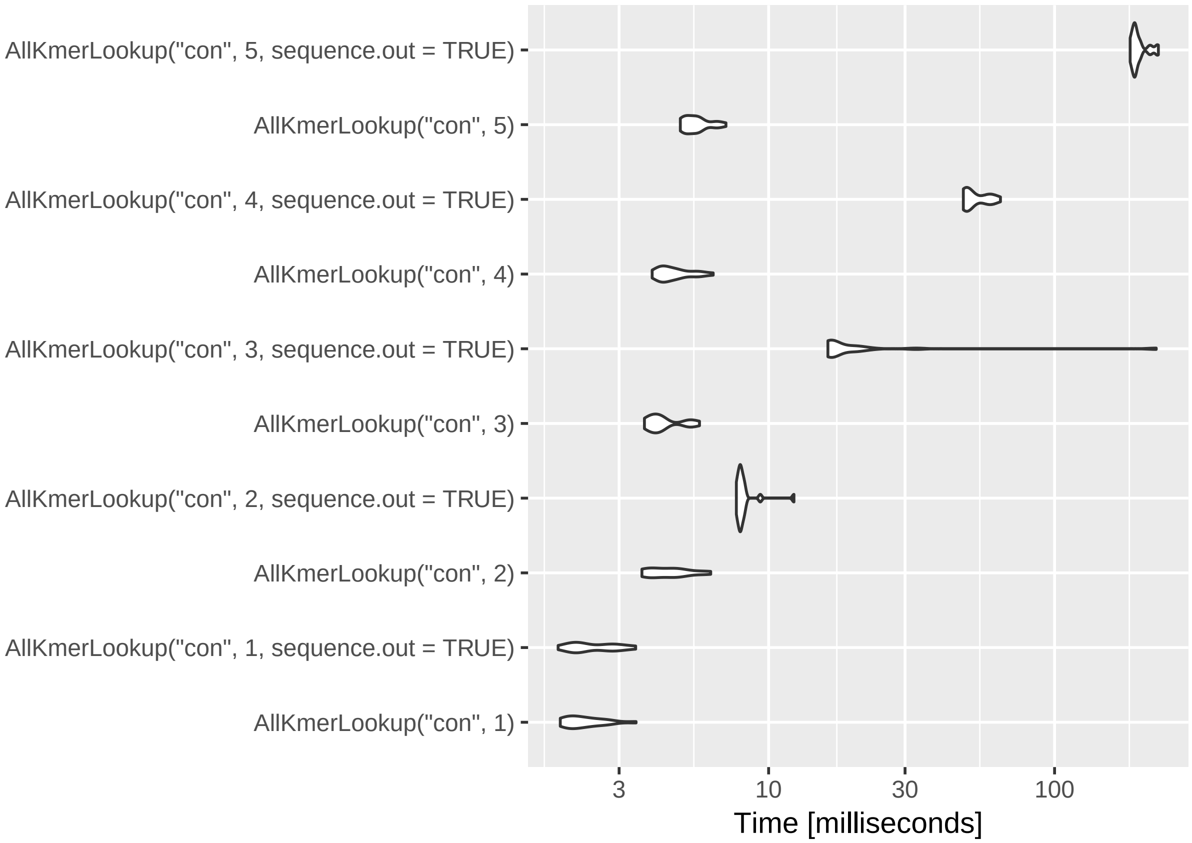
```
FALSE Unit: milliseconds
FALSE                             expr      min       lq     mean   median
FALSE       AllKmerLookup("dnase", 4) 3.919518 4.130370 4.541840 4.437062
FALSE  AllKmerLookup("dnaserigid", 4) 3.891980 4.055586 4.444487 4.499967
FALSE         AllKmerLookup("con", 4) 3.921678 4.100402 4.544324 4.376587
FALSE    AllKmerLookup("conrigid", 4) 3.940036 4.348240 8.309063 4.507796
FALSE         AllKmerLookup("nuc", 4) 3.897380 4.266707 4.987922 4.500237
FALSE    AllKmerLookup("nucrigid", 4) 3.904939 4.193274 5.001934 4.467840
FALSE        uq       max neval cld
FALSE  4.813680  5.694882    20   a
FALSE  4.766163  5.198125    20   a
FALSE  4.909522  5.566373    20   a
FALSE  4.751855 78.813120    20   a
FALSE  4.583659 15.632712    20   a
FALSE  4.741866 14.676996    20   a
```

Number of consecutive trinucleotides



```
FALSE Unit: milliseconds
FALSE                     expr       min        lq       mean    median
FALSE  AllKmerLookup("con", 1)  1.815862  1.974608   2.134628  2.018884
FALSE  AllKmerLookup("con", 2)  3.292633  3.407642   3.691139  3.523192
FALSE  AllKmerLookup("con", 3)  3.396843  3.491336   3.659703  3.570978
FALSE  AllKmerLookup("con", 4)  3.598786  3.751592   4.112475  3.908718
FALSE  AllKmerLookup("con", 5)  4.334202  4.557742   5.086885  4.974856
FALSE  AllKmerLookup("con", 6)  7.654911  8.103611  12.662260  8.409225
FALSE  AllKmerLookup("con", 7) 19.961514 20.532243  56.451853 21.567062
FALSE  AllKmerLookup("con", 8) 68.306180 89.619734 161.829188 97.077831
FALSE          uq        max neval cld
FALSE    2.239185   3.076112    50 a
FALSE    3.764011   5.397909    50 a
FALSE    3.714336   5.043159    50 a
FALSE    4.410335   5.978357    50 a
FALSE    5.372531   6.948113    50 a
FALSE    9.413537  53.739875    50 a
FALSE   39.966221 496.320223    50  b
FALSE  116.783675 578.312584    50   c
```

Sequence Out



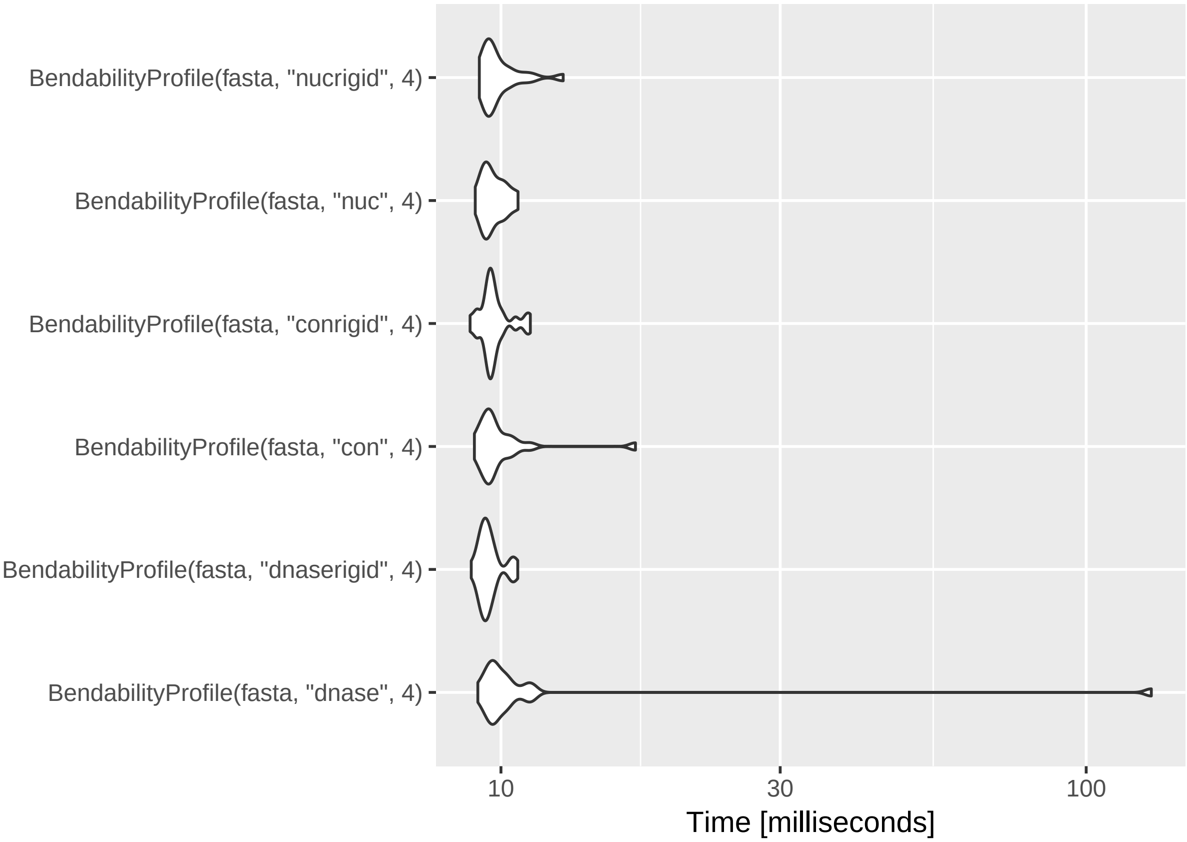
```
## Unit: milliseconds
##                                           expr        min         lq
##                        AllKmerLookup("con", 1)   1.868238   2.005926
##  AllKmerLookup("con", 1, sequence.out = TRUE)   1.835840   2.127955
##                        AllKmerLookup("con", 2)   3.605805   3.846354
##  AllKmerLookup("con", 2, sequence.out = TRUE)   7.712686   7.870891
##                        AllKmerLookup("con", 3)   3.678699   3.914658
##  AllKmerLookup("con", 3, sequence.out = TRUE)  16.118669  16.392156
##                        AllKmerLookup("con", 4)   3.915738   4.220271
##  AllKmerLookup("con", 4, sequence.out = TRUE)  47.972101  48.881380
##                        AllKmerLookup("con", 5)   4.911411   5.130902
##  AllKmerLookup("con", 5, sequence.out = TRUE) 183.746992 189.793923
##        mean     median         uq        max neval  cld
##    2.297176   2.175200   2.498362   3.439499    20 a
##    2.485430   2.178441   2.851761   3.428701    20 a
##    4.536792   4.491058   4.911950   6.273712    20 a
##    8.262844   7.983742   8.166515  12.263948    20 a
##    4.356151   4.140629   4.746186   5.732139    20 a
##   28.872542  16.747715  19.931816 226.734788    20  b
##    4.717757   4.522645   5.022101   6.401141    20 a
##   53.043822  49.896492  58.689892  64.674998    20   c
##    5.626416   5.468642   5.790184   7.092820    20 a
##  197.329989 191.534730 199.069231 230.663484    20    d
```

BendabilityProfile

Splits sequence into k-mers with two-nucleotide overlap and calculates average bendability per k-mer according to the chosen scale.

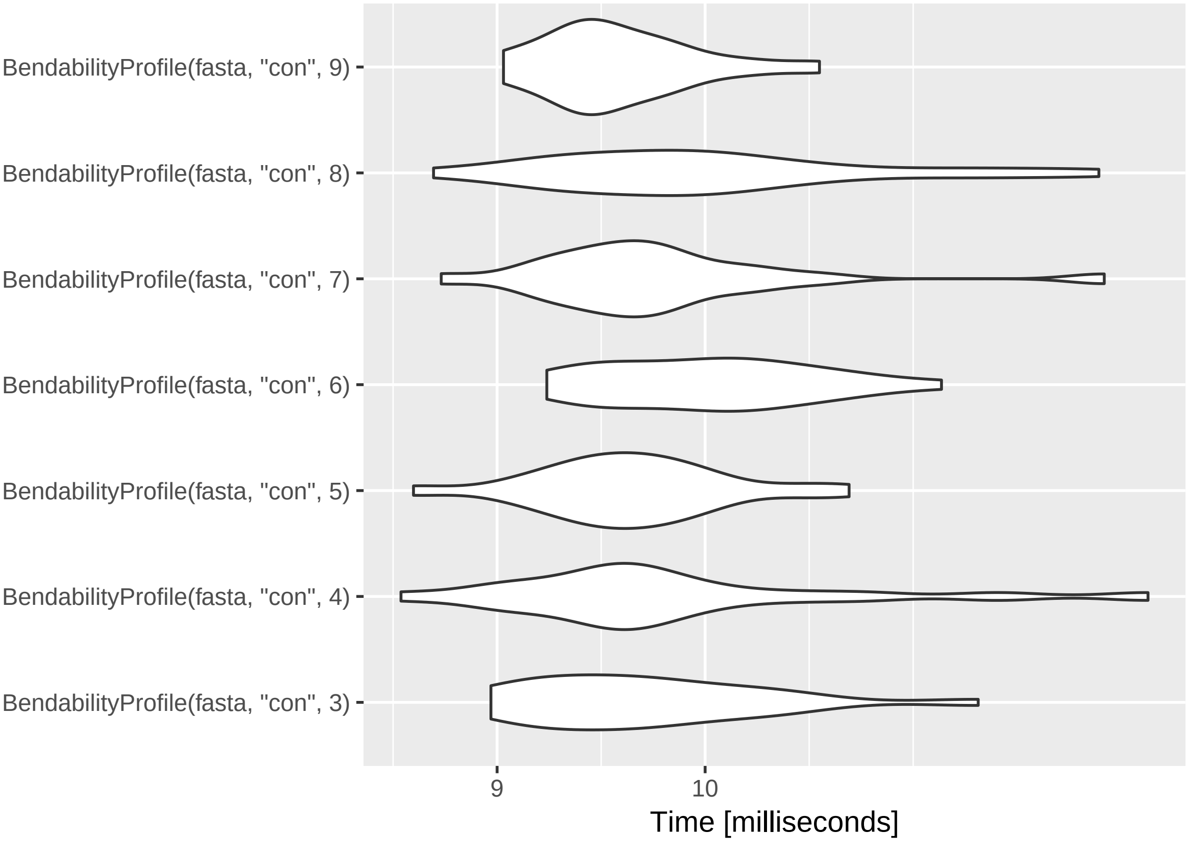
Parameters that can be used include: - Scale - Number of consecutive trinucleotides

Scale



```
## Unit: milliseconds
##                                        expr      min       lq      mean
##       BendabilityProfile(fasta, "dnase", 4) 9.130602 9.634377 15.962650
##  BendabilityProfile(fasta, "dnaserigid", 4) 8.896802 9.239132  9.566047
##         BendabilityProfile(fasta, "con", 4) 9.007492 9.419476 10.090880
##    BendabilityProfile(fasta, "conrigid", 4) 8.855766 9.464292  9.752816
##         BendabilityProfile(fasta, "nuc", 4) 9.037729 9.366831  9.724036
##    BendabilityProfile(fasta, "nucrigid", 4) 9.184597 9.444045  9.949656
##    median        uq       max neval cld
##  9.773955 10.373842 129.20961    20   a
##  9.443504  9.696742  10.68351    20   a
##  9.602520 10.142203  16.97557    20   a
##  9.613589  9.873576  11.22562    20   a
##  9.569853 10.066879  10.69484    20   a
##  9.606840 10.204297  12.77420    20   a
```

Number of consecutive trinucleotides



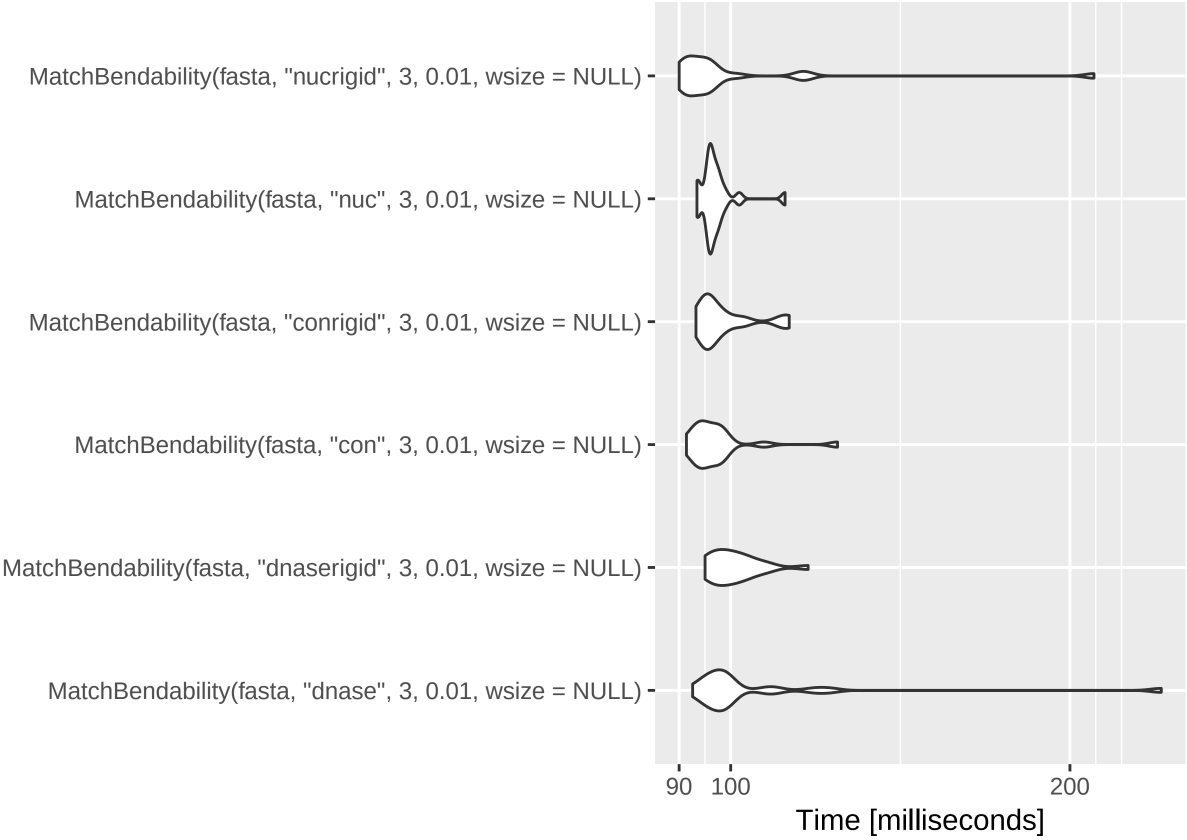
```
## Unit: milliseconds
##                                  expr      min       lq      mean    median
##  BendabilityProfile(fasta, "con", 3) 8.971856 9.247501  9.718826  9.665964
##  BendabilityProfile(fasta, "con", 4) 8.572290 9.373040  9.841017  9.651656
##  BendabilityProfile(fasta, "con", 5) 8.626825 9.372501  9.644825  9.626548
##  BendabilityProfile(fasta, "con", 6) 9.229413 9.560134 10.035616 10.003435
##  BendabilityProfile(fasta, "con", 7) 8.748855 9.406787  9.780651  9.695662
##  BendabilityProfile(fasta, "con", 8) 8.714838 9.416237 10.024223  9.907054
##  BendabilityProfile(fasta, "con", 9) 9.029090 9.349283  9.580004  9.482651
##         uq      max neval cld
##  10.073089 11.48317    20   a
##  10.021254 12.51449    20   a
##   9.900304 10.75640    20   a
##  10.338206 11.27151    20   a
##   9.942691 12.24019    20   a
##  10.385992 12.20671    20   a
##   9.778814 10.59603    20   a
```

MatchBendability

Calculates bendability profile of query sequence and finds all other sequences which have similar (or same) profile.

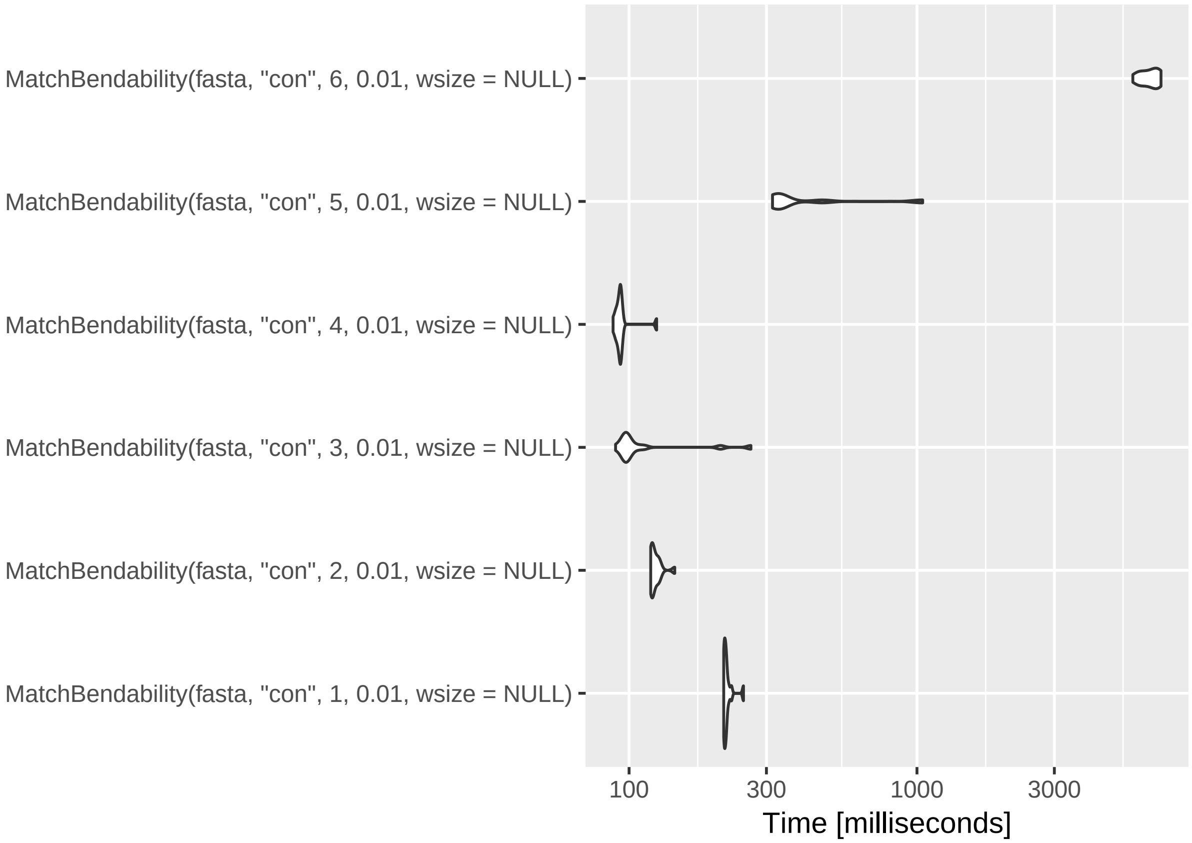
Parameters that can be used include: - Scale - Number of consecutive trinucleotides - Tolerance - wsize - output.list - random.out

Scale



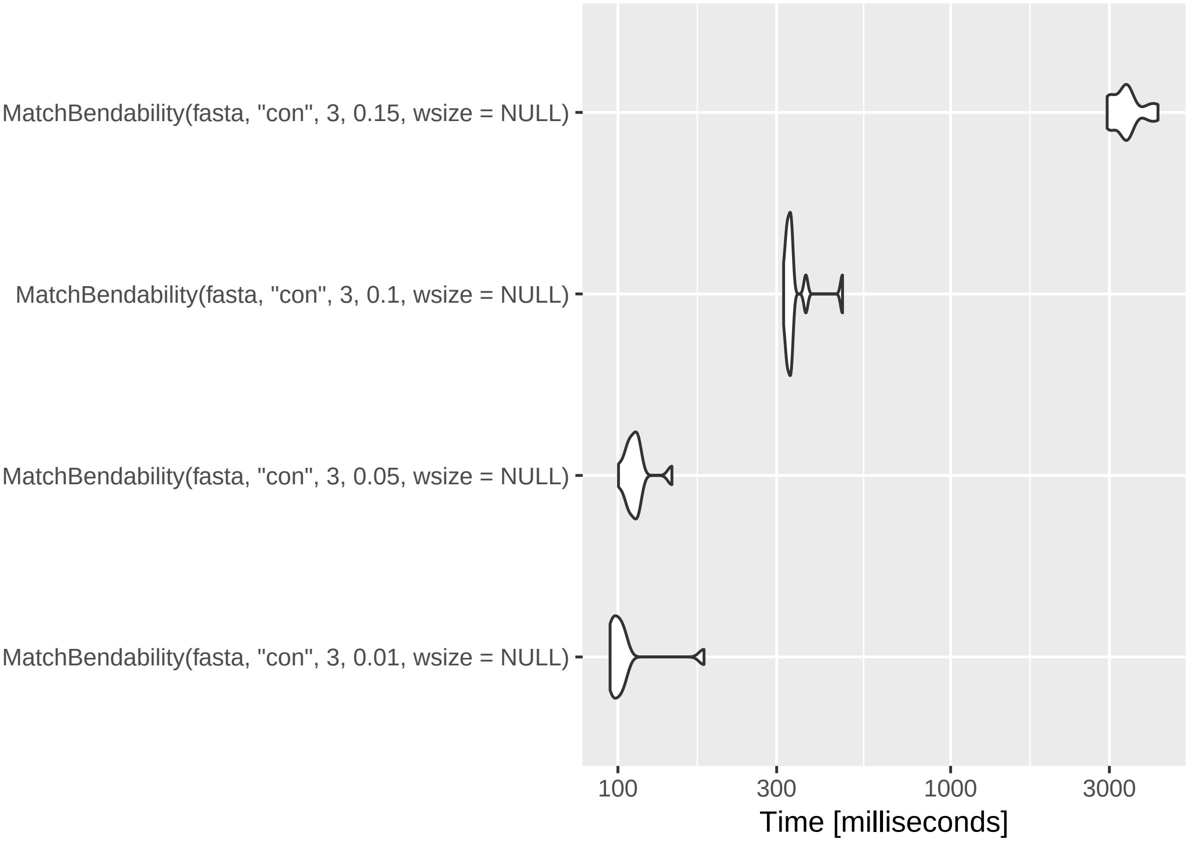
```
## Unit: milliseconds
##                                                          expr      min
##       MatchBendability(fasta, "dnase", 3, 0.01, wsize = NULL) 92.51658
##  MatchBendability(fasta, "dnaserigid", 3, 0.01, wsize = NULL) 94.89831
##         MatchBendability(fasta, "con", 3, 0.01, wsize = NULL) 91.35352
##    MatchBendability(fasta, "conrigid", 3, 0.01, wsize = NULL) 93.14832
##         MatchBendability(fasta, "nuc", 3, 0.01, wsize = NULL) 93.33569
##    MatchBendability(fasta, "nucrigid", 3, 0.01, wsize = NULL) 90.00904
##        lq      mean    median        uq      max neval cld
##  95.59377 107.79314  98.57809 103.62314 241.0360    20   a
##  97.05569 100.96857 100.11398 103.40824 117.1417    20   a
##  93.74119  97.41295  95.41694  98.13425 124.3916    20   a
##  95.04707  98.80212  96.14722 100.22009 112.7022    20   a
##  95.55678  97.13291  96.07109  97.41557 111.7502    20   a
##  91.48095 101.79910  94.43827  96.40991 210.0697    20   a
```

Number of consecutive sequences



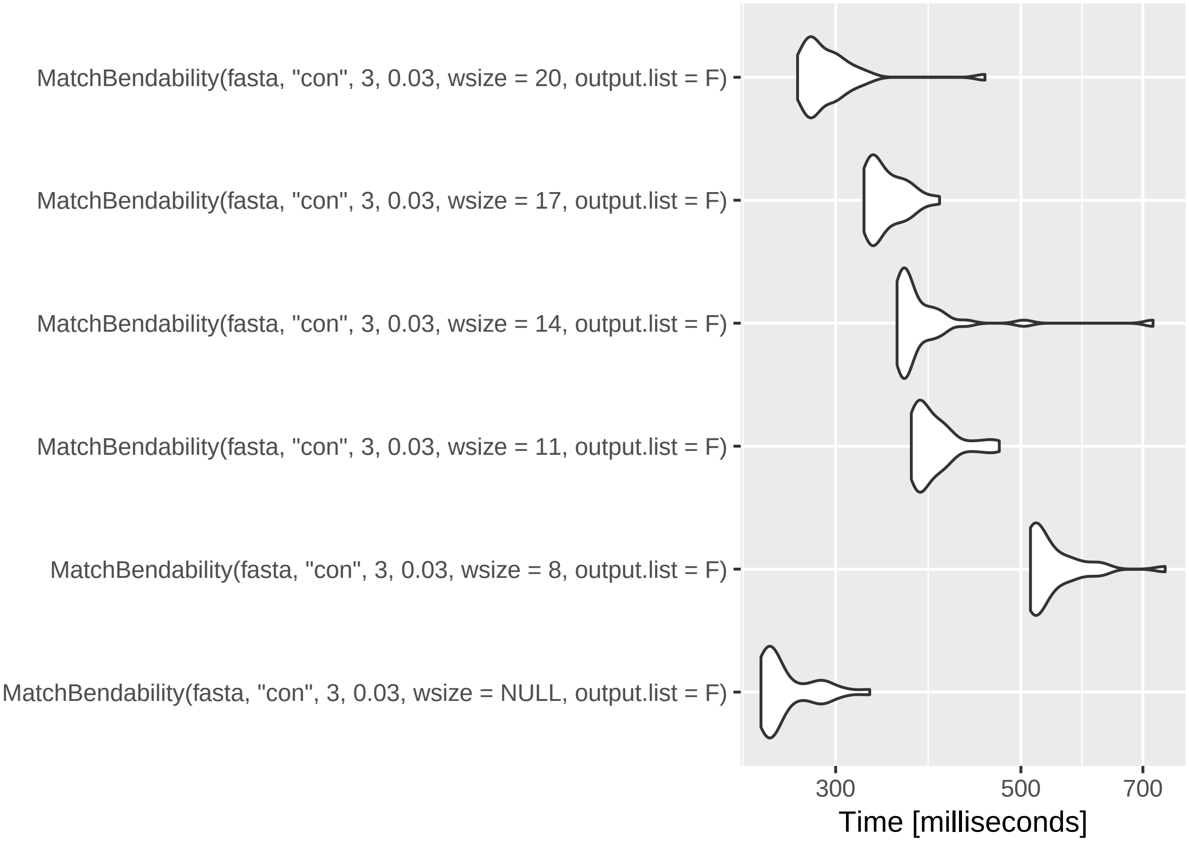
```
## Unit: milliseconds
##                                                   expr        min
##  MatchBendability(fasta, "con", 1, 0.01, wsize = NULL)  213.17010
##  MatchBendability(fasta, "con", 2, 0.01, wsize = NULL)  118.89705
##  MatchBendability(fasta, "con", 3, 0.01, wsize = NULL)   89.76066
##  MatchBendability(fasta, "con", 4, 0.01, wsize = NULL)   88.00581
##  MatchBendability(fasta, "con", 5, 0.01, wsize = NULL)  314.94795
##  MatchBendability(fasta, "con", 6, 0.01, wsize = NULL) 5620.04823
##          lq       mean     median         uq       max neval cld
##   214.02511  218.98269  216.34286  218.38172  249.6871    15 ab
##   119.94537  123.76159  121.10006  125.90240  144.1236    15 a
##    96.04112  117.32280   99.31945  104.19306  264.9813    15 a
##    91.31789   94.42945   93.07327   93.76252  124.6805    15 a
##   326.96000  443.49845  332.88355  403.64166 1046.6390    15  b
##  6033.04322 6430.73386 6513.14677 6781.04809 7039.0110    15   c
```

Tolerance



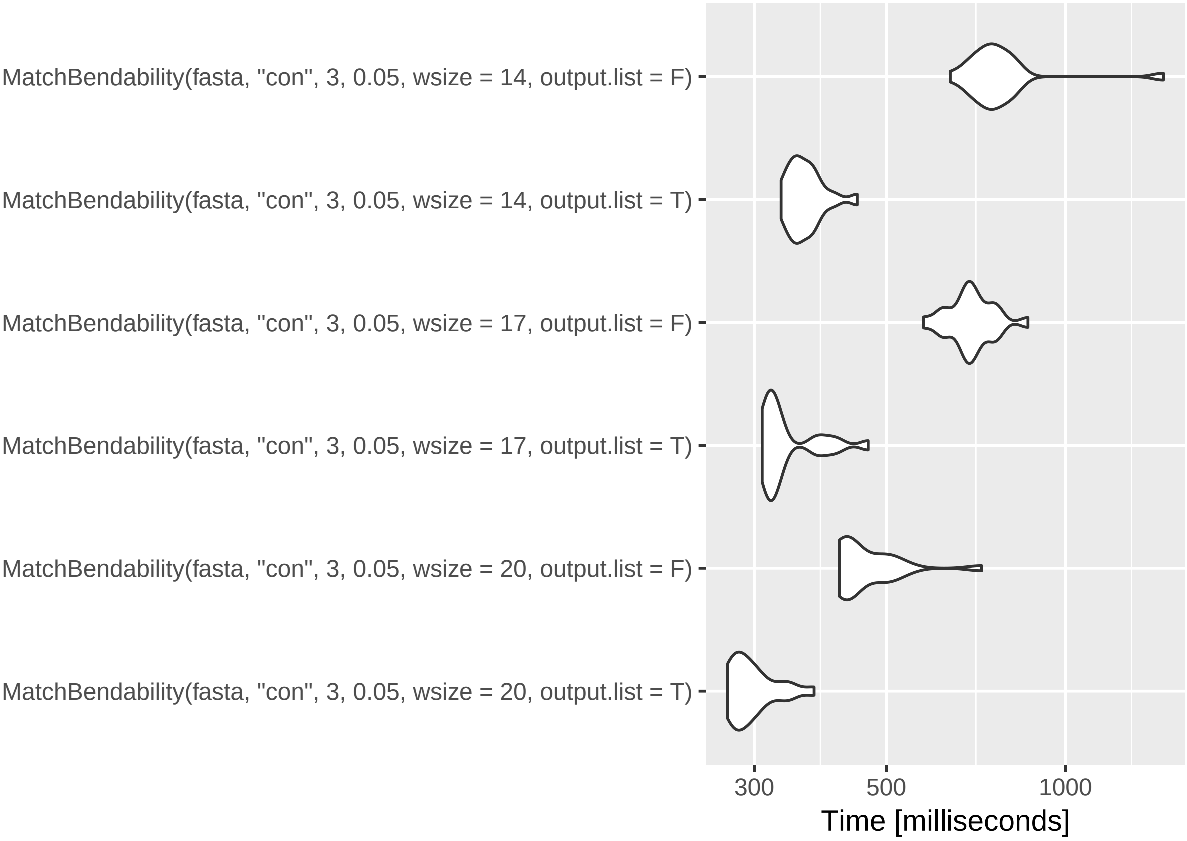
```
## Unit: milliseconds
##                                                    expr        min
##  MatchBendability(fasta, "con", 3, 0.01, wsize = NULL)   94.72823
##  MatchBendability(fasta, "con", 3, 0.05, wsize = NULL)  100.40961
##   MatchBendability(fasta, "con", 3, 0.1, wsize = NULL)  314.82052
##  MatchBendability(fasta, "con", 3, 0.15, wsize = NULL) 2953.85780
##          lq      mean     median        uq       max neval cld
##    95.39993  107.5737   99.94444  104.3010  181.4328    10  a 
##   107.13310  113.6325  111.76481  115.2027  145.3245    10  a 
##   322.60717  344.8043  330.04691  333.7000  473.2135    10  a 
##  3054.20801 3406.8254 3362.35606 3474.8965 4199.7447    10   b
```

Window size



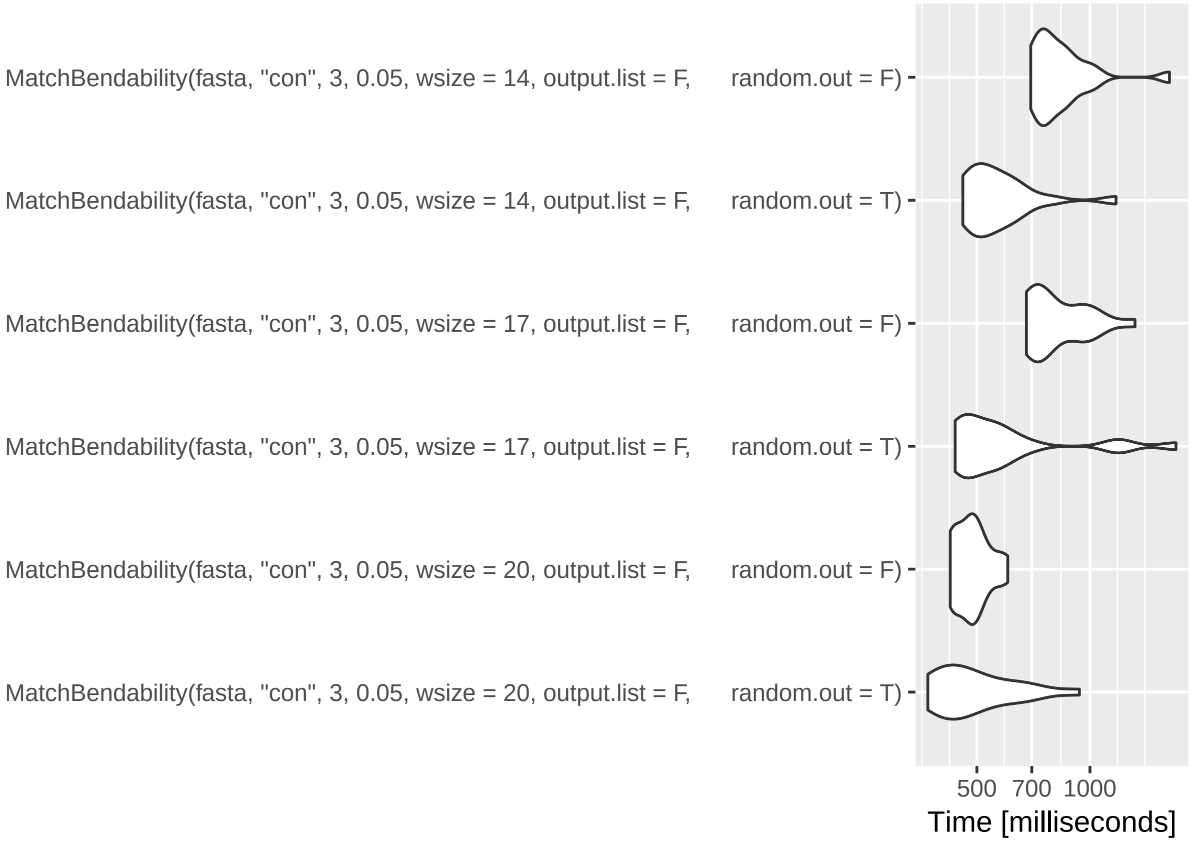
```
## Unit: milliseconds
##                                                                    expr
##  MatchBendability(fasta, "con", 3, 0.03, wsize = NULL, output.list = F)
##     MatchBendability(fasta, "con", 3, 0.03, wsize = 8, output.list = F)
##    MatchBendability(fasta, "con", 3, 0.03, wsize = 11, output.list = F)
##    MatchBendability(fasta, "con", 3, 0.03, wsize = 14, output.list = F)
##    MatchBendability(fasta, "con", 3, 0.03, wsize = 17, output.list = F)
##    MatchBendability(fasta, "con", 3, 0.03, wsize = 20, output.list = F)
##       min       lq     mean   median       uq      max neval   cld
##  244.1812 248.5392 262.5597 252.7967 271.9979 329.5461    30 a
##  513.3709 515.8028 547.4515 530.0222 561.9142 744.3189    30     e
##  369.6090 375.5787 395.4637 385.9496 404.6659 471.0974    30    d
##  355.3656 360.8180 388.4465 365.5680 387.7665 719.8790    30    d
##  324.3923 330.8091 345.7495 339.4505 357.8996 399.5229    30   c
##  270.0865 279.0945 295.6261 285.1169 300.9691 452.8319    30  b
```

Output List



```
## Unit: milliseconds
##                                                                      expr
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 20, output.list = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 20, output.list = F)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 17, output.list = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 17, output.list = F)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 14, output.list = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 14, output.list = F)
##       min       lq     mean   median       uq       max neval  cld
##  270.6281 277.8643 298.8592 290.6919 307.5168  377.9696    20 a
##  417.1378 425.4082 467.1603 435.7913 493.8248  722.9810    20  b
##  309.2946 317.1653 342.8729 323.4957 356.0437  466.0667    20 a
##  577.5178 667.0139 697.3933 688.5150 733.6146  864.6614    20   c
##  332.7561 350.3564 366.5674 362.1495 376.9642  446.7877    20 a
##  640.3478 713.9341 785.1070 752.0359 802.7059 1460.2552    20    d
```

Random Out



```
## Unit: milliseconds
##                                                                                        expr
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 20, output.list = F,      random.out = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 20, output.list = F,      random.out = F)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 17, output.list = F,      random.out = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 17, output.list = F,      random.out = F)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 14, output.list = F,      random.out = T)
##  MatchBendability(fasta, "con", 3, 0.05, wsize = 14, output.list = F,      random.out = F)
##       min       lq     mean   median       uq       max neval cld
##  370.1209 409.2126 509.7598 472.7507 567.2708  937.5145    20  a
##  424.6685 442.3714 486.6252 484.5398 509.3196  604.2903    20  a
##  437.6301 465.1447 645.3722 539.9174 609.3383 1694.5142    20  a
##  677.4220 710.4433 830.8216 763.5334 938.7872 1318.0219    20   b
##  458.7838 491.0835 587.6018 543.2046 627.1972 1173.5770    20  a
##  695.6092 744.5702 853.0123 790.6196 873.9008 1628.3651    20   b
```

ClusterAndConsensus

Intended to present output of function MatchBendability in a more human-friendly format. The output can contain very large numbers of highly similar sequences, so clustering and calculating a consensus can help provide a clearer picture. DISCLAIMER: due to the nature of bendability problem and limitations of IUPAC extended genetic alphabet, output of this function is not intended for further machine use. Not all sequences which can be inferred from consensus output will have satisfied the initial bendability requirements (for example AA/TT will be marked as WW, same as AT/TA).

Parameters that can be used include: - Cutoff - sample.seq

Cutoff

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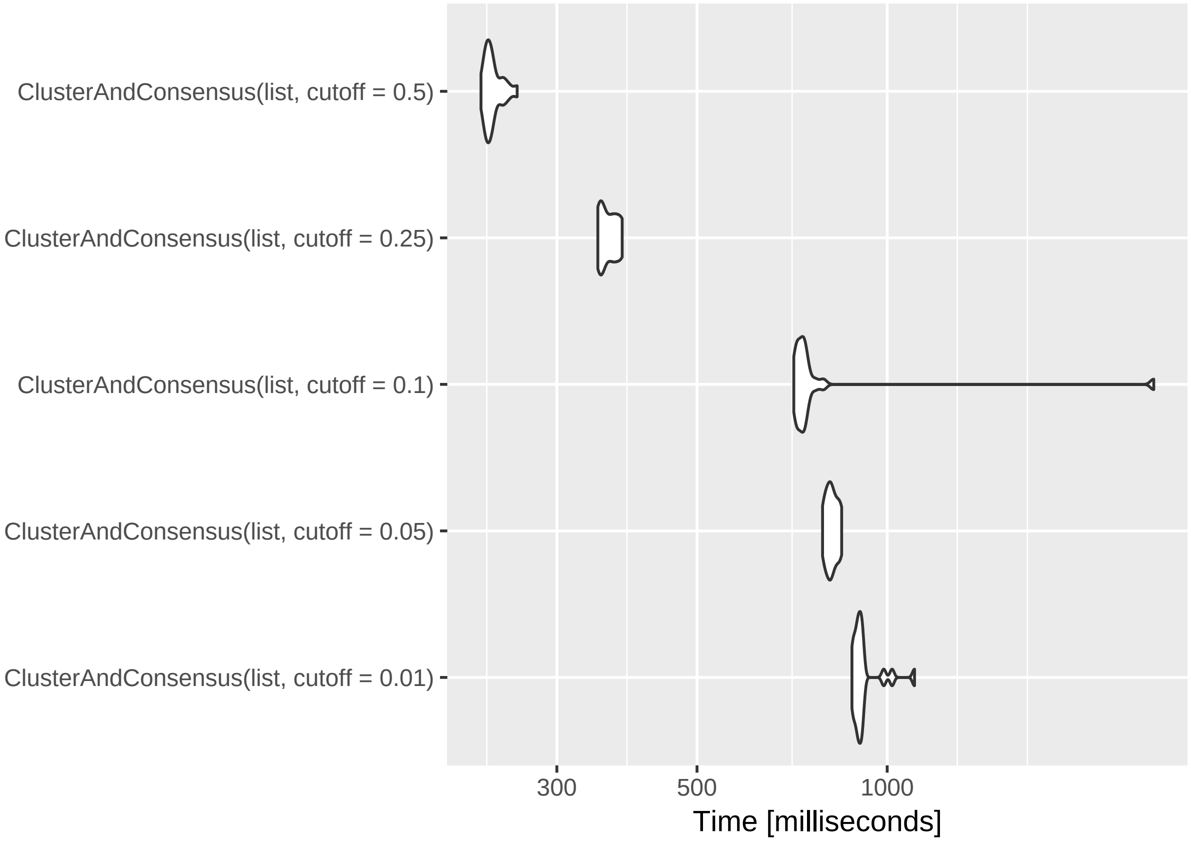

```
## Unit: milliseconds
##                                       expr      min       lq     mean
##  ClusterAndConsensus(list, cutoff = 0.01) 879.4863 893.0848 920.1664
##  ClusterAndConsensus(list, cutoff = 0.05) 790.1144 803.7156 817.3361
##   ClusterAndConsensus(list, cutoff = 0.1) 711.4730 718.9919 830.8027
##  ClusterAndConsensus(list, cutoff = 0.25) 348.3419 351.7409 362.2762
##   ClusterAndConsensus(list, cutoff = 0.5) 227.5318 231.8292 237.6747
##    median       uq       max neval cld
##  903.0080 913.3711 1104.8399    20   b
##  815.4793 831.3965  847.1934    20   b
##  735.3835 743.0333 2641.9503    20   b
##  359.8545 371.7647  380.6694    20  a
##  235.5897 240.7449  259.6222    20  a
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Sample.seq

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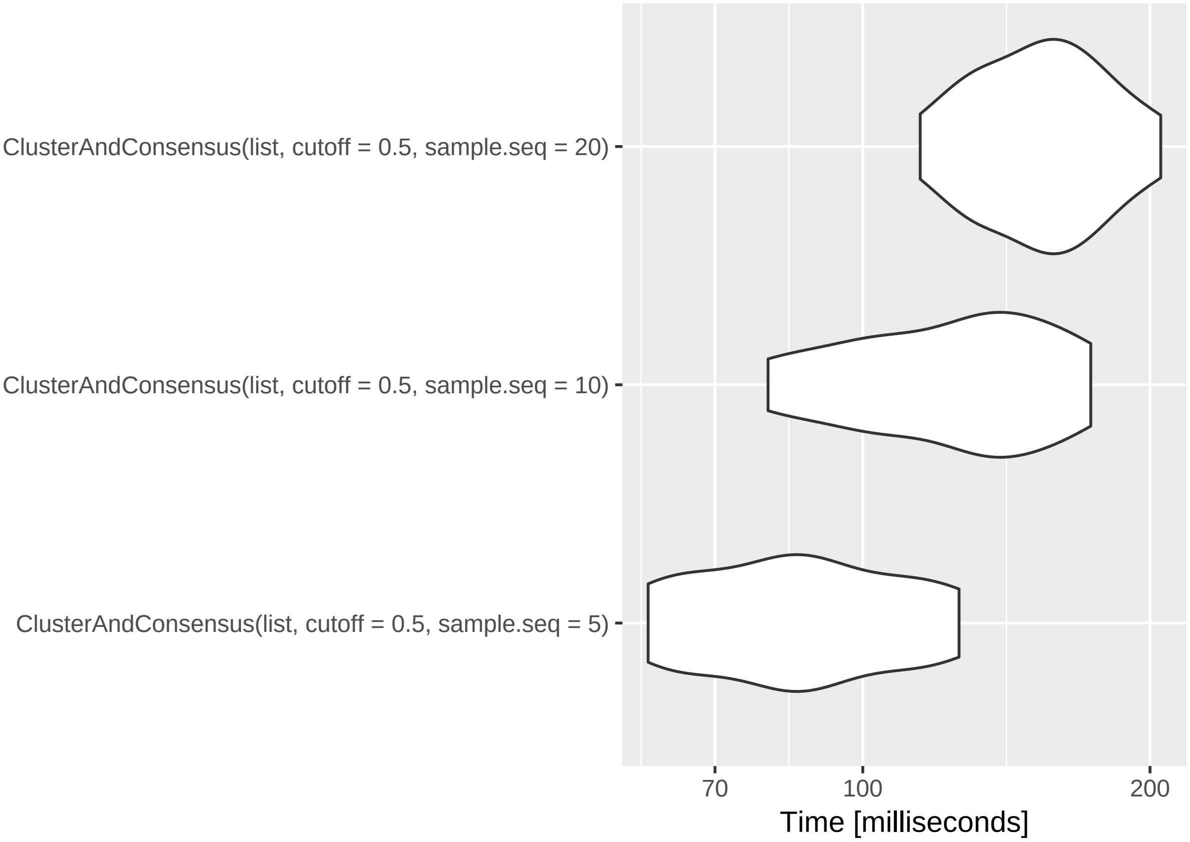

```
## Unit: milliseconds
##                                                       expr       min
##   ClusterAndConsensus(list, cutoff = 0.5, sample.seq = 5)  59.56813
##  ClusterAndConsensus(list, cutoff = 0.5, sample.seq = 10)  79.56527
##  ClusterAndConsensus(list, cutoff = 0.5, sample.seq = 20) 114.86360
##        lq      mean    median       uq      max neval cld
##   68.6882  87.92426  86.12624 106.1674 126.1475    20 a
##  103.1893 126.69119 131.33648 147.4662 173.3567    20  b
##  134.0257 155.34378 154.00721 170.6218 205.2474    20   c
```