

# Package ‘geomeTriD’

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**Type** Package

**Title** A R/Bioconductor package for interactive 3D plot of epigenetic data or single cell data

**Version** 1.5.0

## Description

The geomeTriD (Three-Dimensional Geometry) Package provides interactive 3D visualization of chromatin structures using the WebGL-based 'three.js' (<https://threejs.org/>) or the rgl rendering library. It is designed to identify and explore spatial chromatin patterns within genomic regions. The package generates dynamic 3D plots and HTML widgets that integrate seamlessly with Shiny applications, enabling researchers to visualize chromatin organization, detect spatial features, and compare structural dynamics across different conditions and data types.

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**Imports** aricode, BiocGenerics, Biostrings, clue, cluster, dbscan, future.apply, Seqinfo, GenomicRanges, graphics, grDevices, grid, htmlwidgets, igraph, InteractionSet, IRanges, MASS, Matrix, methods, plotrix, progressr, RANN, rgl, rjson, S4Vectors, scales, stats, trackViewer

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**Author** Jianhong Ou [aut, cre] (ORCID: <<https://orcid.org/0000-0002-8652-2488>>),  
Kenneth Poss [aut, fnd]  
**Maintainer** Jianhong Ou <jou@morgridge.org>

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---

|                   |                                                                   |
|-------------------|-------------------------------------------------------------------|
| geomeTriD-package | <i>Interactive 3D plot of epigenetic data or single cell data</i> |
|-------------------|-------------------------------------------------------------------|

---

Description

The geomeTriD (Three-Dimensional Geometry) Package provides interactive 3D visualization of chromatin structures using the WebGL-based three.js or the rgl rendering library. It is designed to identify and explore spatial chromatin patterns within genomic regions. The package generates dynamic 3D plots and HTML widgets that integrate seamlessly with Shiny applications, enabling researchers to visualize chromatin organization, detect spatial features, and compare structural dynamics across different conditions and data types.

**Author(s)**

**Maintainer:** Jianhong Ou <jou@morgridge.org> ([ORCID](#))

Authors:

- Kenneth Poss <kposs@morgridge.org> [funder]

**See Also**

Useful links:

- <https://github.com/jianhong/geomeTriD>
- Report bugs at <https://github.com/jianhong/geomeTriD/issues>

**Examples**

```
if(interactive()){
  ## quick start from a simple data
  library(geomeTriD)
  set.seed(123)
  obj <- GRanges("1", IRanges(seq.int(10), width = 1),
                 x = sample.int(10, 10),
                 y = sample.int(10, 10),
                 z = sample.int(10, 10)
  )
  feature.gr <- GRanges("1", IRanges(c(3, 7), width = 3),
                       label = c("gene1", "gene2"),
                       col = c("red", "blue"),
                       type = "gene"
  )
  view3dStructure(obj, feature.gr,
                 renderer = "threejs",
                 coor_mark_interval = 5, coor_tick_unit = 2
  )
}
```

---

alignCoor

*Aligns two sets of genomic with x,y,z*


---

**Description**

Aligns two sets of points via rotations and translations by Kabsch Algorithm.

**Usage**

```
alignCoor(query, subject)
```

**Arguments**

query, subject   GRanges objects to alignment.

**Value**

A GRanges object of query aligned to subject.

**Examples**

```
x <- readRDS(system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds",
  package = "geomeTriD"
))
res <- alignCoor(x, x)
A <- view3dStructure(x, k = 3, renderer = "none")
B <- view3dStructure(res, k = 3, renderer = "none")
B <- lapply(B, function(.ele) {
  .ele$side <- "right"
  .ele
})
threeJsViewer(c(A, B))
```

---

autoK

*Automate Cluster Number Selection*


---

**Description**

Automate cluster number selection using Silhouette Width

**Usage**

```
autoK(d, hc, max_k)
```

**Arguments**

|       |                  |
|-------|------------------|
| d     | A dist object.   |
| hc    | A hclust object. |
| max_k | The maximal k.   |

**Value**

The best k number.

**Examples**

```
x <- matrix(rnorm(100), nrow = 5)
d <- dist(x)
hc <- hclust(d)
autoK(d, hc)
```

---

|                     |                             |
|---------------------|-----------------------------|
| availableGeometries | <i>Available Geometries</i> |
|---------------------|-----------------------------|

---

**Description**

The Geometries supported by [threeJsGeometry](#) class

**Usage**

```
availableGeometries
```

**Format**

An object of class character of length 18.

**Examples**

```
availableGeometries
```

---

|              |                                          |
|--------------|------------------------------------------|
| cellClusters | <i>cluster single cell 3D structures</i> |
|--------------|------------------------------------------|

---

**Description**

Perform Hierarchical clustering for given 3D structures.

Calculate distance for each pair of cells after alignment.

**Usage**

```
cellClusters(  
  xyzs,  
  TADs,  
  distance_method = "NID",  
  cluster_method = "ward.D2",  
  rescale = TRUE,  
  quiet = FALSE,  
  parallel = FALSE,  
  ...  
)  
  
cellDistance(  
  xyzs,  
  TADs,  
  distance_method = c("NID", "RMSD", "SRD", "DSDC", "NMI", "ARI", "AMI"),  
  eps,
```

```

    k,
    rescale = TRUE,
    quiet = FALSE,
    parallel = FALSE,
    ...
)

```

## Arguments

|                              |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
|------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>xyzs</code>            | A list of data.frame with x, y, z coordinates or output of <code>cellDistance</code> .                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <code>TADs</code>            | A list of index vectors, where each vector represents a TAD. For example, if the first TAD spans the 2nd to 4th coordinates and the second spans the 8th to 10th coordinates, the list would be: <code>list(c(2, 3, 4), c(8, 9, 10))</code> .                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <code>distance_method</code> | 'SRD', 'DSDC', 'RMSD', 'NMI', 'ARI', 'NID', or 'AMI'. SRD method will first perform clustering and then calculate the Sequence Relabeling Distance <a href="#">SRD</a> . DSDC method will calculate the Euclidean distance of <a href="#">SDC</a> . RMSD method will first do alignment for each cell x, y, z coordinates and then calculate Root Mean Square Deviation (RMSD, the square root of the mean of squared Euclidean distance between corresponding points). ARI, NID, NMI, and AMI method will first perform clustering and then calculate the Adjusted Rand Index (ARI), Normalized information distance (NID), Normalized Mutual Information (NMI), Adjusted Mutual Information (AMI). |
| <code>cluster_method</code>  | The agglomeration method to be used for <a href="#">hclust</a> . Default is 'ward.D2'.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <code>rescale</code>         | Re-scale the object to similar size.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| <code>quiet</code>           | Print the message or not.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <code>parallel</code>        | Run parallel by future or not.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <code>...</code>             | not used.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <code>eps</code>             | numeric or 'auto'. The size (radius) of the epsilon neighborhood. If <code>eps</code> is set, use DBSCAN to cluster the points for each cell.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <code>k</code>               | numeric or 'auto'. The number of groups. If <code>k</code> is set, use <code>hclust</code> to cluster the points for each cell.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

## Value

`cellClusters` return an object of class `hclust`.

`cellDistance` return distance matrix as an object of 'dist'

## Examples

```

set.seed(1)
xyzs <- lapply(seq.int(20), function(i){
  matrix(sample.int(100, 60, replace = TRUE),
    nrow=20, dimnames=list(NULL, c('x', 'y', 'z')))
})
cd <- cellDistance(xyzs, distance_method='RMSD')
cc <- cellClusters(cd)

```

```
# plot(cc)
cutree(cc, k=3)
cd2 <- cellDistance(xyzs, distance_method='SRD', eps=40)
```

---

```
create3dGenomicSignals
```

*create 3d Geometry by given genomic signals*

---

## Description

Create a 3d Geometry by given genomic signals for target 3d positions.

## Usage

```
create3dGenomicSignals(
  GenoSig,
  targetObj,
  signalTransformFun,
  positionTransformFun,
  genomicScoreRange,
  reverseGenomicSigs,
  type = "segment",
  tag,
  name,
  color = c("gray30", "darkred"),
  rotation = c(0, 0, 0),
  ...
)
```

## Arguments

|                      |                                                                                                                                                                                               |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| GenoSig              | The Genomic signals. An object of <a href="#">GRanges</a> , <a href="#">Pairs</a> , or <a href="#">GInteractions</a> with scores or an object of <a href="#">track</a> .                      |
| targetObj            | The GRanges object with mcols x0, y0, z0, x1, y1, and z1                                                                                                                                      |
| signalTransformFun   | The transformation function for genomic signals.                                                                                                                                              |
| positionTransformFun | The transformation function for the coordinates. The function must have input as a data.frame with colnames x0, y0, z0, x1, y1, and z1. And it must have output as same dimension data.frame. |
| genomicScoreRange    | The genomic signals range.                                                                                                                                                                    |
| reverseGenomicSigs   | Plot the genomic signals in reverse values.                                                                                                                                                   |
| type                 | The Geometry type. See <a href="#">threeJsGeometry</a>                                                                                                                                        |

|          |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| tag      | The tag used to group geometries.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| name     | The prefix for the name of the geometries.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| color    | The color of the signal. If there is metadata 'color' in GenoSig this parameter will be ignored.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| rotation | The rotations in the x, y and z axis in radians.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| ...      | the parameters for each different type of geometries. If type is 'segments', lwd.maxGenomicSigs (the maximal lwd of the line) is required. If type is 'circle', radius (the radius of the circle) and the maxVal (the value for 2*pi) is required. If type is 'sphere', 'dodecahedron', 'icosahedron', 'octahedron', or 'tetrahedron', radius is required. If type is 'box', 'capsule', 'cylinder', 'cone', or 'torus', if the properties of correspond geometry is not set, they will be set to the transformed score value. If type is 'json', please refer the documentation about BufferGeometryLoader at threejs.org If input 'GenoSig' is an object of Pairs or GInteractions, the type will be set to 'polygon' and topN is used to set how many top events will be plot. |

### Value

[threeJsGeometry](#) objects or NULL

### Examples

```
library(GenomicRanges)
GenoSig <- GRanges("chr1", IRanges(seq(1, 100, by = 10), width = 10),
  score = seq.int(10)
)
pos <- matrix(rnorm(303), ncol = 3)
pos <- cbind(
  x0 = pos[seq.int(100), 1],
  x1 = pos[seq.int(101)[-1], 1],
  y0 = pos[seq.int(100), 2],
  y1 = pos[seq.int(101)[-1], 2],
  z0 = pos[seq.int(100), 3],
  z1 = pos[seq.int(101)[-1], 3]
)
targetObj <- GRanges("chr1", IRanges(seq.int(100), width = 1))
mcols(targetObj) <- pos
ds <- create3dGenomicSignals(GenoSig, targetObj,
  signalTransformFun = function(x) {
    log2(x + 1)
  },
  reverseGenomicSigs = FALSE,
  type = "segment",
  lwd.maxGenomicSigs = 8,
  name = "test",
  tag = "test"
)
threeJsViewer(ds)
```

---

createTADGeometries     *create 3d Geometry by given TADs*

---

## Description

Create a 3d Geometry by given TADs for target 3d positions.

## Usage

```
createTADGeometries(
  tad,
  targetObj,
  type = "sphere",
  name = "TAD_",
  tag = "TAD",
  alpha = 0.2,
  lwd = 3,
  ...
)
```

## Arguments

|           |                                                                             |
|-----------|-----------------------------------------------------------------------------|
| tad       | The TAD. An object of <a href="#">GRanges</a> .                             |
| targetObj | The GRanges object with mcols x0, y0, z0, x1, y1, and z1                    |
| type      | The Geometry type. default is sphere. Possible types are sphere or segment. |
| name      | The prefix for the name of the geometries.                                  |
| tag       | The tag used to group geometries.                                           |
| alpha     | alpha value. default is 0.2                                                 |
| lwd       | line width for segment.                                                     |
| ...       | other properties.                                                           |

## Value

[threeJsGeometry](#) objects

## Examples

```
library(GenomicRanges)
obj <- readRDS(system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds",
  package = "geomeTriD"
))
tjg <- view3dStructure(obj, renderer = "none")
pc <- pointCluster(as.data.frame(mcols(obj)))
tads <- split(obj, pc$cluster)
tads <- tads[names(tads)!="0"] # cluster 0 is noise
tads <- unlist(range(GRangesList(tads)))
```

```
backbone <- extractBackbonePositions(tjg)
tad_geometries <- createTADGeometries(tads, backbone)
threeJsViewer(tjg, tad_geometries)
```

---

`extractBackbonePositions`

*Extract the backbone coordinates from output of mdsPlot*

---

### Description

Extract the positions from output of `mdsPlot` and used as the 'targetObj' for function `create3dGenomicSignals`

### Usage

```
extractBackbonePositions(v3d_output, n = "backbone")
```

### Arguments

|                         |                                                                                           |
|-------------------------|-------------------------------------------------------------------------------------------|
| <code>v3d_output</code> | The output of <code>mdsPlot</code> or <code>view3dStructure</code> for <code>k=3</code> . |
| <code>n</code>          | The backbone name of in the inputs.                                                       |

### Value

An `GRanges` object with positions of `x0`, `x1`, `y0`, `y1`, `z0` and `z1`.

### Examples

```
library(GenomicRanges)
gi_nij <- readRDS(system.file("extdata", "nij.chr6.51120000.53200000.gi.rds",
                             package = "geomeTriD"))
range_chr6 <- GRanges("chr6", IRanges(51120000, 53200000))
geos <- mdsPlot(gi_nij, range = range_chr6, k = 3, render = "none")
extractBackbonePositions(geos)
```

---

`fill_NA`

*fill NA values by upstream and downstream points*

---

### Description

Fill NA values by previous and next points coordinates.

### Usage

```
fill_NA(xyz)
```

**Arguments**

xyz                    A matrix or data.frame with columns 'x', 'y', 'z'

**Value**

A matrix or data.frame.

**Examples**

```
xyz <- matrix(seq.int(21), ncol=3, dimnames=list(NULL, c('x', 'y', 'z')))  
xyz[c(1, 5, 7), ] <- NA  
fill_NA(xyz)
```

---

|              |                      |
|--------------|----------------------|
| gaussianBlur | <i>Gaussian blur</i> |
|--------------|----------------------|

---

**Description**

Do Gaussian for the distance matrix.

**Usage**

```
gaussianBlur(mat, size = 5, sigma = 1, ...)
```

**Arguments**

|       |                           |
|-------|---------------------------|
| mat   | A matrix.                 |
| size  | The kernel size           |
| sigma | The strength of the blur. |
| ...   | Not used.                 |

**Value**

A matrix.

**Examples**

```
mat <- matrix(runif(100), 10, 10)  
blurred_mat <- gaussianBlur(mat, size = 5, sigma = 1)
```

---

|                 |                           |
|-----------------|---------------------------|
| loopBouquetPlot | <i>plot GInteractions</i> |
|-----------------|---------------------------|

---

## Description

plot graph for GInteractions

## Usage

```
loopBouquetPlot(  
  gi,  
  range,  
  feature.gr,  
  genomicSigs,  
  signalTransformFun = function(x) {  
    log2(x + 1)  
  },  
  label_region = FALSE,  
  show_edges = TRUE,  
  show_cluster = TRUE,  
  lwd.backbone = 2,  
  col.backbone = "gray",  
  lwd.maxGenomicSigs = 8,  
  reverseGenomicSigs = TRUE,  
  col.backbone_background = "gray70",  
  alpha.backbone_background = 0.5,  
  lwd.gene = 2,  
  lwd.nodeCircle = 1,  
  col.nodeCircle = "#DDDDDD25",  
  lwd.edge = 2,  
  col.edge = "gray80",  
  coor_mark_interval = 1e+05,  
  col.coor = "black",  
  show_coor = TRUE,  
  coor_tick_unit = 1000,  
  label_gene = TRUE,  
  col.tension_line = "black",  
  lwd.tension_line = 1,  
  length.arrow = NULL,  
  safe_text_force = 3,  
  method = 1,  
  doReduce = FALSE,  
  ...  
)
```

## Arguments

|    |                                            |
|----|--------------------------------------------|
| gi | An object of <a href="#">GInteractions</a> |
|----|--------------------------------------------|

|                                                                                                          |                                                                                                                                                           |
|----------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>range</code>                                                                                       | The region to plot. an object of <a href="#">GRanges</a>                                                                                                  |
| <code>feature.gr</code>                                                                                  | The annotation features to be added. An object of <a href="#">GRanges</a> .                                                                               |
| <code>genomicSigs</code>                                                                                 | The genomic signals. An object of <a href="#">GRanges</a> with scores or an object of <a href="#">track</a> .                                             |
| <code>signalTransformFun</code>                                                                          | The transformation function for genomic signals.                                                                                                          |
| <code>label_region</code>                                                                                | Label the region node or not.                                                                                                                             |
| <code>show_edges</code>                                                                                  | Plot the interaction edges or not.                                                                                                                        |
| <code>show_cluster</code>                                                                                | Plot the cluster background or not.                                                                                                                       |
| <code>lwd.backbone, lwd.gene, lwd.nodeCircle, lwd.edge, lwd.tension_line, lwd.maxGenomicSigs</code>      | Line width for the linker, gene, interaction node circle, the dashed line of interaction edges, the tension line and the maximal reversed genomic signal. |
| <code>col.backbone, col.backbone_background, col.nodeCircle, col.edge, col.tension_line, col.coor</code> | Color for the DNA chain, the compact DNA chain, the node circle, the linker, the tension line and the coordinates marker.                                 |
| <code>reverseGenomicSigs</code>                                                                          | Plot the Genomic signals in reverse values.                                                                                                               |
| <code>alpha.backbone_background</code>                                                                   | Alpha channel for transparency of backbone background.                                                                                                    |
| <code>coor_mark_interval</code>                                                                          | The coordinates marker interval. Numeric(1). Set to 0 to turn it off. The default value 1e5 means show coordinates every 0.1M bp.                         |
| <code>show_coor</code>                                                                                   | Show coordinates or not.                                                                                                                                  |
| <code>coor_tick_unit</code>                                                                              | The bps for every ticks. Default is 1K.                                                                                                                   |
| <code>label_gene</code>                                                                                  | Show gene symbol or not.                                                                                                                                  |
| <code>length.arrow</code>                                                                                | Length of the edges of the arrow head (in inches).                                                                                                        |
| <code>safe_text_force</code>                                                                             | The loops to avoid the text overlapping.                                                                                                                  |
| <code>method</code>                                                                                      | Plot method. Could be 1 or 2.                                                                                                                             |
| <code>doReduce</code>                                                                                    | Reduce the GInteractions or not.                                                                                                                          |
| <code>...</code>                                                                                         | Parameter will be passed to <a href="#">layout_with_fr</a> .                                                                                              |

**Value**

A invisible list with the key points of the plot.

**Examples**

```
library(InteractionSet)
gi <- readRDS(system.file("extdata", "gi.rds", package = "trackViewer"))
range <- GRanges("chr2", IRanges(234500000, 235000000))
library(TxDb.Hsapiens.UCSC.hg19.knownGene)
library(org.Hs.eg.db)
```

```

feature.gr <- genes(TxDb.Hsapiens.UCSC.hg19.knownGene)
feature.gr <- subsetByOverlaps(feature.gr, range(regions(gi)))
symbols <- mget(feature.gr$gene_id, org.Hs.egSYMBOL, ifnotfound = NA)
feature.gr$label[lengths(symbols) == 1] <- unlist(symbols[lengths(symbols) == 1])
feature.gr$col <- sample(1:7, length(feature.gr), replace = TRUE)
feature.gr$type <- sample(c("cRE", "gene"),
  length(feature.gr),
  replace = TRUE,
  prob = c(0.1, 0.9)
)
feature.gr$pch <- rep(NA, length(feature.gr))
feature.gr$pch[feature.gr$type == "cRE"] <- 11
loopBouquetPlot(gi, range, feature.gr)

```

---

mdsPlot

---

*Plot genomic interactions by multi-dimensional scaling plot*


---

## Description

This function will convert the interactions scores into a distance matrix and then plot the matrix by multi-dimensional scaling plot.

## Usage

```

mdsPlot(
  gi,
  range,
  feature.gr,
  k = 2,
  genomicSigs,
  signalTransformFun = function(x) {
    log2(x + 1)
  },
  lwd.backbone = 2,
  col.backbone = "gray",
  lwd.maxGenomicSigs = 8,
  reverseGenomicSigs = TRUE,
  col.backbone_background = if (k == 2) "gray70" else c("white", "darkred"),
  alpha.backbone_background = 0.5,
  lwd.gene = 3,
  coor_mark_interval = 5e+05,
  col.coor = "black",
  show_coor = TRUE,
  coor_tick_unit = 50000,
  label_gene = TRUE,
  col.tension_line = "black",
  lwd.tension_line = 1,
  length.arrow = NULL,

```

```

    safe_text_force = 3,
    square = TRUE,
    renderer = c("rgl", "threejs", "none", "granges"),
    ...
)

```

## Arguments

|                                                                                |                                                                                                                                                                                                                                                                                            |
|--------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>gi</code>                                                                | An object of <a href="#">GInteractions</a>                                                                                                                                                                                                                                                 |
| <code>range</code>                                                             | The region to plot. an object of <a href="#">GRanges</a>                                                                                                                                                                                                                                   |
| <code>feature.gr</code>                                                        | The annotation features to be added. An object of <a href="#">GRanges</a> .                                                                                                                                                                                                                |
| <code>k</code>                                                                 | The dimension of plot. 2: 2d, 3: 3d.                                                                                                                                                                                                                                                       |
| <code>genomicSigs</code>                                                       | The genomic signals. An object of <a href="#">GRanges</a> with scores or an object of <a href="#">track</a> .                                                                                                                                                                              |
| <code>signalTransformFun</code>                                                | The transformation function for genomic signals.                                                                                                                                                                                                                                           |
| <code>lwd.backbone, lwd.gene, lwd.tension_line, lwd.maxGenomicSigs</code>      | Line width for the linker, gene, interaction node circle, the dashed line of interaction edges, the tension line and the maximal reversed genomic signal.                                                                                                                                  |
| <code>col.backbone, col.backbone_background, col.tension_line, col.coor</code> | Color for the DNA chain, the compact DNA chain, the node circle, the linker, the tension line and the coordinates marker.                                                                                                                                                                  |
| <code>reverseGenomicSigs</code>                                                | Plot the genomic signals in reverse values.                                                                                                                                                                                                                                                |
| <code>alpha.backbone_background</code>                                         | Alpha channel for transparency of backbone background.                                                                                                                                                                                                                                     |
| <code>coor_mark_interval</code>                                                | The coordinates marker interval. Numeric(1). Set to 0 to turn it off. The default value 1e5 means show coordinates every 0.1M bp.                                                                                                                                                          |
| <code>show_coor</code>                                                         | Plot ticks in the line to show the DNA compact tension.                                                                                                                                                                                                                                    |
| <code>coor_tick_unit</code>                                                    | The bps for every ticks. Default is 1K.                                                                                                                                                                                                                                                    |
| <code>label_gene</code>                                                        | Show gene symbol or not.                                                                                                                                                                                                                                                                   |
| <code>length.arrow</code>                                                      | Length of the edges of the arrow head (in inches).                                                                                                                                                                                                                                         |
| <code>safe_text_force</code>                                                   | The loops to avoid the text overlapping.                                                                                                                                                                                                                                                   |
| <code>square</code>                                                            | A logical value that controls whether control points for the curve are created city-block fashion or obliquely. See <a href="#">grid.curve</a> .                                                                                                                                           |
| <code>renderer</code>                                                          | The renderer of the 3D plots. Could be <code>rgl</code> or <code>threejs</code> . The <code>threejs</code> will create a <code>htmlwidgets</code> . If 'none' is set, a list of object will be returned. If 'granges' is set, A <a href="#">GRanges</a> with coordinates will be returned. |
| <code>...</code>                                                               | Parameter will be passed to <a href="#">isoMDS</a> .                                                                                                                                                                                                                                       |

## Value

Coordinates for 2d or 3d.

**Examples**

```

library(InteractionSet)
gi <- readRDS(system.file("extdata", "nij.chr6.51120000.53200000.gi.rds",
  package = "geomeTriD"
))
range <- GRanges("chr6", IRanges(51120000, 53200000))
library(TxDb.Hsapiens.UCSC.hg19.knownGene)
library(org.Hs.eg.db)
feature.gr <- genes(TxDb.Hsapiens.UCSC.hg19.knownGene)
feature.gr <- subsetByOverlaps(feature.gr, range(regions(gi)))
symbols <- mget(feature.gr$gene_id, org.Hs.egSYMBOL, ifnotfound = NA)
feature.gr$label[lengths(symbols) == 1] <- unlist(symbols[lengths(symbols) == 1])
feature.gr$col <- sample(1:7, length(feature.gr), replace = TRUE)
feature.gr$type <- sample(c("cRE", "gene"),
  length(feature.gr),
  replace = TRUE,
  prob = c(0.1, 0.9)
)
mdsPlot(gi, range, feature.gr)

```

pointCluster

*Perform DBSCAN clustering***Description**

Perform DBSCAN clustering for given 3D coordinates.

**Usage**

```
pointCluster(xyz, eps = "auto", quiet = FALSE, ...)
```

**Arguments**

|       |                                                                     |
|-------|---------------------------------------------------------------------|
| xyz   | A data.frame with x, y, z coordinates                               |
| eps   | The size (radius) of the epsilon neighborhood. Default 'auto'.      |
| quiet | Print message or not.                                               |
| ...   | other parameters could be used by dbscan function except x and eps. |

**Value**

An object of class `dbscan_fast`.

**Examples**

```

xyz <- readRDS(system.file('extdata', '4DNFI1UEG1HD.chr21.FLAMINGO.res.rds',
  package='geomeTriD'))
pc <- pointCluster(xyz)

```

---

|           |                                                 |
|-----------|-------------------------------------------------|
| rglViewer | <i>rgl Viewer View the 3d structure by rgl.</i> |
|-----------|-------------------------------------------------|

---

**Description**

rgl Viewer View the 3d structure by rgl.

**Usage**

```
rglViewer(..., background = "gray")
```

**Arguments**

|            |                                |
|------------|--------------------------------|
| ...        | objects of threeJsGeometry.    |
| background | background of the main camera. |

**Value**

MULL

**Examples**

```
obj <- readRDS(system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds",
  package = "geomeTriD"
))
feature.gr <- readRDS(system.file("extdata", "4DNFI1UEG1HD.feature.gr.rds",
  package = "geomeTriD"
))
tjg <- view3dStructure(obj,
  k = 3, feature.gr = feature.gr, renderer = "none",
  length.arrow = grid::unit(0.000006, "native")
)
if(interactive()){
  rglViewer(tjg, background = 'white')
}
```

---

|     |                             |
|-----|-----------------------------|
| SDC | <i>Distance to centroid</i> |
|-----|-----------------------------|

---

**Description**

Calculates the mean of distance from each point to the geometric center (centroid)

**Usage**

```
SDC(xyz)
```

**Arguments**

xyz                      A data.frame with x, y, z coordinates.

**Value**

The mean of squared Euclidean distance to the centroid.

**Examples**

```
xyz <- matrix(seq.int(12), ncol = 3, dimnames=list(NULL, c('x', 'y', 'z')))
SDC(xyz)
```

---

|                |                                                       |
|----------------|-------------------------------------------------------|
| smooth3dPoints | <i>Calculate the smoothed curve for input GRanges</i> |
|----------------|-------------------------------------------------------|

---

**Description**

This function will do smooth for given resolution (tile) for inputs and it is important step to prepare the inputs for [create3dGenomicSignals](#) and [view3dStructure](#).

**Usage**

```
smooth3dPoints(obj, resolution = 30, ...)
```

**Arguments**

obj                      GRanges object with mcols x, y, and z  
resolution              number of points at which to evaluate the smooth curve.  
...                      parameters passed to [splinefun](#)

**Value**

GRanges object with smoothed points of x0, y0, z0, x1, y1, and z1.

**Examples**

```
library(GenomicRanges)
obj <- GRanges("1", IRanges(seq.int(5) * 10, width = 10),
  x = seq.int(5), y = seq.int(5), z = seq.int(5)
)
smooth3dPoints(obj, 5)
```

---

spatialDistanceMatrix *Create the spatial distance matrix*


---

## Description

Create the spatial distance matrix for given 3D coordinates.

boundaryScore calculate the boundary score for a distance matrix. Please note that, this boundary score is the reverse of insulation score because we are using the distance matrix but not the interaction matrix.

boundaryScoreTAD assign the TAD boundaries via boundary score.

hierarchicalClusteringTAD assign the TAD boundaries via hierarchical clustering.

compartment calculate the compartment by principal component analysis.

spatialDistanceHeatmap will use base R to plot the spatial distance matrix.

## Usage

```
spatialDistanceMatrix(xyz, output = "matrix", fill_NA = FALSE, ...)
```

```
boundaryScore(spatialDistances, window = 5, background = 10, ...)
```

```
boundaryScoreTAD(
  spatialDistances,
  bin_size,
  window = 5,
  Z_cutoff = 2.3,
  norm = FALSE,
  boundaryScores,
  ...
)
```

```
hierarchicalClusteringTAD(spatialDistances, bin_size, window = 5, k, ...)
```

```
compartment(xyz.gr, genome, minWidth = 1)
```

```
spatialDistanceHeatmap(
  spatialDistances,
  components = c("compartment", "boundaryScoreTAD", "hierarchicalClusteringTAD"),
  col = hcl.colors(n = 12, "OrRd"),
  at = seq(0, 1, length.out = 2),
  label_unit = "M",
  window = 5,
  background = 10,
  d_cutoff = Inf,
  Z_cutoff = 2.3,
  norm = FALSE,
```

```

    Gaussian_blur = FALSE,
    useRaster = FALSE,
    ...
)

```

## Arguments

|                  |                                                                                          |
|------------------|------------------------------------------------------------------------------------------|
| xyz              | A GRanges object with x, y, z coordinates                                                |
| output           | "matrix" or "dist".                                                                      |
| fill_NA          | Fill the missing value or not.                                                           |
| ...              | Parameters could be used by downstream function.                                         |
| spatialDistances | The output of spatialDistanceMatrix or the input of spatialDistanceMatrix.               |
| window           | The window size for boundary score.                                                      |
| background       | The background window size for local background.                                         |
| bin_size         | The bin size.                                                                            |
| Z_cutoff         | The Z_cutoff value for boundary.                                                         |
| norm             | Normalize the boundary score or not.                                                     |
| boundaryScores   | The output of boundaryScore.                                                             |
| k                | The cluster number. The final TAD numbers will be no greater than this number.           |
| xyz.gr           | A GRanges object with x,y,z coordinates.                                                 |
| genome           | A BSgenome object                                                                        |
| minWidth         | The minimal width of input region.                                                       |
| components       | The components to plot.                                                                  |
| col              | a list of colors such as that generated by hcl.colors, gray.colors or similar functions. |
| at               | The label position of X, and Y axis.                                                     |
| label_unit       | unit for labels. 'M', 1e6; 'K', 1e3, 'G', 1e9.                                           |
| d_cutoff         | The maximal cutoff value of distance matrix.                                             |
| Gaussian_blur    | Do Gaussian blur or not.                                                                 |
| useRaster        | logical; if TRUE a bitmap raster is used to plot the image instead of polygons.          |

## Value

A matrix of Euclidean distance with fixed bins.

boundaryScore return a data frame with the boundary score and the Z scores.

boundaryScoreTAD return a list of the index or the positions of coordinates.

hierarchicalClusteringTAD return a list of the index or the positions of coordinates.

compartment return a GRanges object with A,B annotations.

**Examples**

```

xyz.gr <- readRDS(system.file('extdata', '4DNFI1UEG1HD.chr21.FLAMINGO.res.rds',
  package='geomeTriD'))
bin_size <- 5000 #width(xyz.gr)[1]
sdm <- spatialDistanceMatrix(xyz.gr)
spatialDistanceHeatmap(sdm)
head(boundaryScoreTAD(sdm, bin_size=bin_size))
head(hierarchicalClusteringTAD(sdm, bin_size=bin_size))
library(BSgenome.Hsapiens.UCSC.hg19)
compartment(xyz.gr, genome=BSgenome.Hsapiens.UCSC.hg19)

```

---

SRD

---

*Sequence Relabeling Distance*


---

**Description**

Compares two cluster sequences after best label alignment.

**Usage**

```
SRD(c1, c2, noise = 0)
```

**Arguments**

|        |                                       |
|--------|---------------------------------------|
| c1, c2 | The cluster sequence 1 and 2.         |
| noise  | The noise cluster name. Default is 0. |

**Value**

The mean value of hamming distance after label alignment.

**Examples**

```

c1 <- c(-1, 0, 1, 1, -1, 3, 3, 5, 5, 5) # `-1` is noise
c2 <- c(-1, 4, 4, 4, -1, 2, 2, 2, 2, 2) # `-1` is noise
SRD(c1, c2, noise=-1)

```

---

```
threeJsGeometry-class  Class "threeJsGeometry"
```

---

### Description

An object of class "threeJsGeometry" represents 'three.js' geometry.

### Usage

```
threeJsGeometry(...)

## S4 method for signature 'threeJsGeometry'
x$name

## S4 replacement method for signature 'threeJsGeometry'
x$name <- value

## S4 method for signature 'threeJsGeometry'
show(object)
```

### Arguments

|        |                                                                  |
|--------|------------------------------------------------------------------|
| ...    | Each argument in ... becomes an slot in the new threeJsGeometry. |
| x      | an object of threeJsGeometry                                     |
| name   | slot name of threeJsGeometry                                     |
| value  | value to be assigned                                             |
| object | an object of threeJsGeometry                                     |

### Slots

x,y,z "numeric", specify the x, y, and z coordinates.  
 rotation "numeric", specify the rotations in the x, y and z axis in radians.  
 colors "character", the colors for each geometry.  
 type "character", the type of the geometry. See [availableGeometries](#).  
 side 'character', the side for side by side plot in [threeJsViewer](#).  
 layer 'character', the two layer plot in [threeJsViewer](#).  
 tag 'character', the tag used to group geometries.  
 properties A "list", the properties to control the geometry.

### Examples

```
tjg <- threeJsGeometry()
```

---

|               |                                                           |
|---------------|-----------------------------------------------------------|
| threeJsViewer | <i>threeJs Viewer The htmlwidgets viewer for threeJs.</i> |
|---------------|-----------------------------------------------------------|

---

## Description

threeJs Viewer The htmlwidgets viewer for threeJs.

## Usage

```
threeJsViewer(
  ...,
  background = c("#33333388", "#444444DD", "#444444DD", "#33333388"),
  maxRadius = 1,
  maxLineWidth = 50,
  title = NULL,
  width = NULL,
  height = NULL
)
```

## Arguments

|               |                                                 |
|---------------|-------------------------------------------------|
| ...           | objects of threeJsGeometry.                     |
| background    | background of the main camera (left and right). |
| maxRadius     | max value of the controls for radius.           |
| maxLineWidth  | max value of the controls for line width.       |
| title         | the titles of the plot.                         |
| width, height | width and height of the widgets.                |

## Details

We convert data frames to JSON by `getOption("shiny.json.digits", 7)` to avoid the error "Uncaught SyntaxError: Expected ',' or ']' after array element in JSON" for json parse process when handling big data. User can change the option 'shiny.json.digits' larger or smaller number to increase or decrease the digits when converting numbers.

## Value

A htmlwidgets widget.

## Examples

```
library(GenomicRanges)
flamingo <- system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds", package = "geomeTriD")
x <- readRDS(flamingo[[1]])
## resize to bigger value to get better init view
mcols(x) <- as.data.frame(mcols(x)) * 1e5
```

```

set.seed(1)
line <- threeJsGeometry(
  x = x$x, y = x$y, z = x$z,
  colors = sample(palette(), length(x), replace = TRUE),
  type = "line",
  properties = list(size = 4)
)
sphere <- x[sample.int(length(x), 100)]
sphere <- threeJsGeometry(
  x = sphere$x, y = sphere$y, z = sphere$z,
  colors = "red",
  type = "sphere",
  properties = list(radius = 0.08)
)
torus <- x[sample.int(length(x), 100)]
torus <- threeJsGeometry(
  x = torus$x, y = torus$y, z = torus$z,
  colors = "blue",
  type = "torus",
  properties = list(
    radius = 0.08,
    tube = 0.03
  )
)
cylinder <- x[sample.int(length(x), 100)]
cylinder <- threeJsGeometry(
  x = cylinder$x, y = cylinder$y, z = cylinder$z,
  colors = "green",
  type = "cylinder",
  properties = list(
    "height" = 0.07,
    "radiusTop" = 0.05,
    "radiusBottom" = 0.09
  )
)
labels <- x[sample.int(length(x), 5)]
fontURL <- paste0('https://raw.githubusercontent.com/mrdoob/three.js/refs/',
  'heads/dev/examples/fonts/helvetiker_regular.typeface.json')
labels <- threeJsGeometry(
  x = labels$x, y = labels$y, z = labels$z,
  colors = "black",
  type = "text",
  properties = list(
    "label" = "text",
    "font" = readLines(fontURL),
    "size" = .5,
    "depth" = .1
  )
)
threeJsViewer(line, sphere, torus, cylinder)

```

---

threeJsViewer-shiny     *Shiny bindings for threeJsViewer*


---

**Description**

Output and render functions for using threeJsViewer within Shiny applications and interactive Rmd documents.

**Usage**

```
threejsOutput(outputId, width = "100%", height = "600px")

renderthreeJsViewer(expr, env = parent.frame(), quoted = FALSE)
```

**Arguments**

|               |                                                                                                                                |
|---------------|--------------------------------------------------------------------------------------------------------------------------------|
| outputId      | output variable to read from                                                                                                   |
| width, height | Must be a valid CSS unit (like '100%', '600px', 'auto') or a number, which will be coerced to a string and have 'px' appended. |
| expr          | An expression that generates a threeJsViewer                                                                                   |
| env           | The environment in which to evaluate expr.                                                                                     |
| quoted        | Is expr a quoted expression (with quote())? This is useful if you want to save an expression in a variable.                    |

**Value**

An output or render function that enables the use of the threeJsViewer widget.

**Examples**

```
if (interactive()) {
  library(GenomicRanges)
  flamingo <- system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds", package = "geomeTriD")
  x <- readRDS(flamingo[[1]])
  ## resize to bigger value to get better init view
  mcols(x) <- as.data.frame(mcols(x)) * 1e5
  line <- threeJsGeometry(
    x = x$x, y = x$y, z = x$z,
    colors = sample(palette(), length(x), replace = TRUE),
    type = "line",
    properties = list(size = 4)
  )
  library(shiny)
  runApp(list(
    ui = bootstrapPage(
      threejsOutput("plot")
    ),
    server = function(input, output) {
```

```

        output$plot <- renderthreeJsViewer({
          threeJsViewer(line)
        })
      }
    })
  }
}

```

view3dCells

*Plot cell xyz data in 2d or 3d***Description**

Plot cell xyz data with grid or rgl package.

**Usage**

```

view3dCells(
  cells,
  x,
  y,
  z,
  color = "blue",
  colorFun = function(x, pal = seq.int(8)) {
    if (is.character(x))
      x <-
        as.numeric(factor(x))
    limits <- range(x)
    pal[findInterval(x, seq(limits[1],
      limits[2], length.out = length(pal) + 1), all.inside = TRUE)]
  },
  shape = "sphere",
  radius = 0.1,
  tag = "cell",
  renderer = c("rgl", "threejs", "none"),
  ...
)

```

**Arguments**

|                      |                                                                                                                                                    |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------|
| cells                | A data.frame.                                                                                                                                      |
| x, y, z              | Column names of x, y, z.                                                                                                                           |
| color, shape, radius | The column names for color, shape, radius or the value(length=1) of them.                                                                          |
| colorFun             | The function to map values into colors.                                                                                                            |
| tag                  | The tag for controller.                                                                                                                            |
| renderer             | The renderer of the 3D plots. Could be rgl or threejs. The threejs will create a htmlwidgets. If 'none' is set, a list of object will be returned. |
| ...                  | Not used.                                                                                                                                          |

**Value**

A list of threeJsGeometry objects or a htmlwidget.

**Examples**

```
cells <- readRDS(system.file("extdata", "pbmc_small.3d.rds",
  package = "geomeTriD"
))
view3dCells(cells,
  x = "umap_1", y = "umap_2", z = "umap_3",
  color = "nCount_RNA",
  renderer = "threejs"
)
```

---

view3dStructure

---

*Plot GRanges xyz data in 2d or 3d*


---

**Description**

Plot GRanges xyz data with grid or rgl package.

**Usage**

```
view3dStructure(
  obj,
  feature.gr,
  genomicSigs,
  region,
  signalTransformFun = function(x) {
    log2(x + 1)
  },
  k = 3,
  renderer = c("rgl", "threejs", "none"),
  lwd.backbone = 2,
  col.backbone = "gray",
  lwd.maxGenomicSigs = 8,
  reverseGenomicSigs = TRUE,
  col.backbone_background = if (k == 2) "gray70" else c("gray30", "darkred"),
  alpha.backbone_background = 0.5,
  lwd.gene = 3,
  coor_mark_interval = 5e+05,
  col.coor = "black",
  show_coor = TRUE,
  coor_tick_unit = 50000,
  label_gene = TRUE,
  col.tension_line = "black",
  lwd.tension_line = 1,
```

```

length.arrow = unit(abs(diff(obj$x))/20, "native"),
safe_text_force = 3,
square = TRUE,
cluster3Dpoints = FALSE,
...
)

```

## Arguments

|                                                                                |                                                                                                                                                                                                          |
|--------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>obj</code>                                                               | GRanges object with mcols x, y, and/or z                                                                                                                                                                 |
| <code>feature.gr</code>                                                        | The annotation features to be added. An object of <a href="#">GRanges</a> .                                                                                                                              |
| <code>genomicSigs</code>                                                       | The Genomic signals. An object of <a href="#">GRanges</a> with scores or an object of <a href="#">track</a> .                                                                                            |
| <code>region</code>                                                            | A GRanges object with the region to be plot.                                                                                                                                                             |
| <code>signalTransformFun</code>                                                | The transformation function for genomic signals.                                                                                                                                                         |
| <code>k</code>                                                                 | The dimension of plot. 2: 2d, 3: 3d.                                                                                                                                                                     |
| <code>renderer</code>                                                          | The renderer of the 3D plots. Could be <code>rgl</code> or <code>threejs</code> . The <code>threejs</code> will create a <code>htmlwidgets</code> . If 'none' is set, a list of object will be returned. |
| <code>lwd.backbone, lwd.gene, lwd.tension_line, lwd.maxGenomicSigs</code>      | Line width for the linker, gene, interaction node circle, the dashed line of interaction edges, the tension line and the maximal reversed genomic signal.                                                |
| <code>col.backbone, col.backbone_background, col.tension_line, col.coor</code> | Color for the DNA chain, the compact DNA chain, the node circle, the linker, the tension line and the coordinates marker.                                                                                |
| <code>reverseGenomicSigs</code>                                                | Plot the genomic signals in reverse values.                                                                                                                                                              |
| <code>alpha.backbone_background</code>                                         | Alpha channel for transparency of backbone background.                                                                                                                                                   |
| <code>coor_mark_interval</code>                                                | The coordinates marker interval. Numeric(1). Set to 0 to turn it off. The default value 1e5 means show coordinates every 0.1M bp.                                                                        |
| <code>show_coor</code>                                                         | Plot ticks in the line to show the DNA compact tension.                                                                                                                                                  |
| <code>coor_tick_unit</code>                                                    | The bps for every ticks. Default is 1K.                                                                                                                                                                  |
| <code>label_gene</code>                                                        | Show gene symbol or not.                                                                                                                                                                                 |
| <code>length.arrow</code>                                                      | Length of the edges of the arrow head (in inches).                                                                                                                                                       |
| <code>safe_text_force</code>                                                   | The loops to avoid the text overlapping.                                                                                                                                                                 |
| <code>square</code>                                                            | A logical value that controls whether control points for the curve are created city-block fashion or obliquely. See <a href="#">grid.curve</a> .                                                         |
| <code>cluster3Dpoints</code>                                                   | A logical value that controls whether cluster the points in 3D. It will be ignored when <code>k=2</code> .                                                                                               |
| <code>...</code>                                                               | Parameters for <a href="#">create3dGenomicSignals</a> .                                                                                                                                                  |

**Value**

Coordinates for 2d or a list of threeJsGeometry objects or a htmlwidget.

**Examples**

```
obj <- readRDS(system.file("extdata", "4DNFI1UEG1HD.chr21.FLAMINGO.res.rds",  
  package = "geomeTriD")  
)  
feature.gr <- readRDS(system.file("extdata", "4DNFI1UEG1HD.feature.gr.rds",  
  package = "geomeTriD")  
)  
tjg <- view3dStructure(obj,  
  k = 3, feature.gr = feature.gr, renderer = "none",  
  length.arrow = grid::unit(0.000006, "native")  
)
```

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