Package ‘mbkmeans’

May 30, 2024

Type  Package
Title  Mini-batch K-means Clustering for Single-Cell RNA-seq
Version  1.20.0
Description  Implements the mini-batch k-means algorithm for large datasets, including support for on-disk data representation.
Depends  R (>= 3.6)
Imports  methods, DelayedArray, Rcpp, S4Vectors, SingleCellExperiment, SummarizedExperiment, ClusterR, benchmarkme, Matrix, BiocParallel
Suggests  beachmat, HDF5Array, Rhdf5lib, BiocStyle, TENxPBMCData, scater, DelayedMatrixStats, bluster, knitr, testthat, rmarkdown
License  MIT + file LICENSE
Encoding  UTF-8
LazyData  true
RoxygenNote  7.1.1
LinkingTo  Rcpp, RcppArmadillo (>= 0.7.2), Rhdf5lib, beachmat, ClusterR
SystemRequirements  C++11
VignetteBuilder  knitr
biocViews  Clustering, GeneExpression, RNASEq, Software, Transcriptomics, Sequencing, SingleCell

BugReports  https://github.com/drisso/mbkmeans/issues
git_url  https://git.bioconductor.org/packages/mbkmeans
git_branch  RELEASE_3_19
git_last_commit  eed13ef
git_last_commit_date  2024-04-30
Repository  Bioconductor 3.19
Date/Publication  2024-05-29
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| blocksize | blocksize |

**Description**

Return the maximum number of rows to use based on the amount of ram memory.

**Usage**

```r
blocksize(data, ram = get_ram())
```

**Arguments**

- `data` : matrix-like object.
- `ram` : the max amount of ram (in bytes) to use.

**Value**

Numeric value of the maximum number of rows.

**Examples**

```r
data <- matrix(NA, nrow = 100, ncol=1000)
blocksize(data, ram=1e6)
```
**clusterRows**

*Cluster rows of a matrix*

**Description**

Cluster rows of a matrix-like object with a variety of algorithms.

**Details**

This function is deprecated. Please use the `clusterRows` function in the `bluster` Bioconductor package.

**compute_wcss**

*Compute Whithin-Cluster Sum of Squares*

**Description**

Given a vector of cluster labels, a matrix of centroids, and a dataset, it computes the WCSS.

**Usage**

```r
compute_wcss(clusters, cent, data)
```

**Arguments**

- `clusters` numeric vector with the cluster assignments.
- `cent` numeric matrix with the centroids (clusters in rows, variables in columns).
- `data` matrix-like object containing the data (numeric or integer).

**Value**

A numeric vector with the value of WCSS per cluster.

**Examples**

```r
data = matrix(1:30,nrow = 10)
c1 <- mini_batch(data, 2, 10, 10)
compute_wcss(c1$Clusters, c1$centroids, data)
```
mbkmeans

Mini-Batch k-means for large single cell sequencing data

Description

This is an implementation of the mini-batch k-means algorithm of Sculley (2010) for large single cell sequencing data with the dimensionality reduction results as input in the reducedDim() slot.

Usage

mbkmeans(x, ...)

## S4 method for signature 'SummarizedExperiment'
mbkmeans(x, whichAssay = 1, ...)

## S4 method for signature 'SingleCellExperiment'
mbkmeans(x, reduceMethod = "PCA", whichAssay = 1, ...)

## S4 method for signature 'LinearEmbeddingMatrix'
mbkmeans(x, ...)

## S4 method for signature 'ANY'
mbkmeans(
  x,
  clusters,
  batch_size = min(500, NCOL(x)),
  max_iters = 100,
  num_init = 1,
  init_fraction = batch_size/NCOL(x),
  initializer = "kmeans++",
  compute_labels = TRUE,
  calc_wcss = FALSE,
  early_stop_iter = 10,
  verbose = FALSE,
  CENTROIDS = NULL,
  tol = 1e-04,
  BPPARAM = BiocParallel::SerialParam(),
  ...
)

Arguments

x

The object on which to run mini-batch k-means. It can be a matrix-like object (e.g., matrix, Matrix, DelayedMatrix, HDF5Matrix) with genes in the rows and samples in the columns. Specialized methods are defined for SummarizedExperiment and SingleCellExperiment.

... passed to 'blockApply'.
whichAssay  The assay to use as input to mini-batch k-means. If x is a SingleCellExperiment, this is ignored unless reduceMethod = NA.
reduceMethod  Name of dimensionality reduction results to use as input to mini-batch k-means. Set to NA to use the full matrix.
clusters  the number of clusters
batch_size  the size of the mini batches. By default, it equals the minimum between the number of observations and 500.
max_iters  the maximum number of clustering iterations
num_init  number of times the algorithm will be run with different centroid seeds
init_fraction  proportion of data to use for the initialization centroids (applies if initializer is \textit{kmeans++}). Should be a float number between 0.0 and 1.0. By default, it uses the relative batch size.
initializer  the method of initialization. One of \textit{kmeans++} and \textit{random}. See details for more information
compute_labels  logical indicating whether to compute the final cluster labels.
calc_wcss  logical indicating whether the per-cluster WCSS is computed. Ignored if ‘compute_labels = FALSE’.
early_stop_iter  continue that many iterations after calculation of the best within-cluster-sum-of-squared-error
verbose  either TRUE or FALSE, indicating whether progress is printed during clustering
CENTROIDS  a matrix of initial cluster centroids. The rows of the CENTROIDS matrix should be equal to the number of clusters and the columns should be equal to the columns of the data
tol  a float number. If, in case of an iteration (iteration > 1 and iteration < max_iters) ‘tol’ is greater than the squared norm of the centroids, then kmeans has converged
BPPARAM  See the ‘BiocParallel’ package. Only the label assignment is done in parallel.

Details
The implementation is largely based on the \texttt{MiniBatchKmeans} function of the \texttt{ClusterR} package. The contribution of this package is to provide support for on-disk data representations such as HDF5, through the use of \texttt{DelayedMatrix} and \texttt{HDF5Matrix} objects, as well as for sparse data representation through the classes of the \texttt{Matrix} package. We also provide high-level methods for objects of class \texttt{SummarizedExperiment}, \texttt{SingleCellExperiment}, and \texttt{LinearEmbeddingMatrix}.
This function performs k-means clustering using mini batches.
\texttt{random}: random selection of data rows as initial centroids

Value
A list with the following attributes: centroids, WCSS_per_cluster, best_initialization, iters_per_initialization.
A list with the following attributes: centroids, WCSS_per_cluster, best_initialization, iters_per_initialization
Author(s)

Lampros Mouselimis and Yuwei Ni

References


https://github.com/mlampros/ClusterR

Examples

```r
library(SummarizedExperiment)
se <- SummarizedExperiment(matrix(rnorm(100), ncol=10))
mbkmeans(se, clusters = 2)
library(SingleCellExperiment)
sce <- SingleCellExperiment(matrix(rnorm(100), ncol=10))
mbkmeans(sce, clusters = 2, reduceMethod = NA)
x<-matrix(rnorm(100), ncol=10)
mbkmeans(x,clusters = 3)
```

MbkmeansParam

**Mini-batch k-means clustering**

Description

Run the mini-batch k-means `mbkmeans` function with the specified number of centers within `clusterRows` from the `bluster` Bioconductor package.

Usage

```r
MbkmeansParam(centers, ...)
```

Arguments

- **centers**
  
  An integer scalar specifying the number of centers. Alternatively, a function that takes the number of observations and returns the number of centers. Note, the `mbkmeans` function uses the argument `clusters` argument to represent this argument. However, we use `centers` to match

- **...**
  
  Further arguments to pass to `mbkmeans`.

Details

This function is deprecated. Please use the `MbkmeansParam` function in the `bluster` Bioconductor package.
**mini_batch**

---

**mini_batch**  
*Mini_batch*

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**Description**

Mini-batch-k-means for matrix-like objects

**Usage**

```r
mini_batch(
  data,
  clusters,
  batch_size,
  max_iters,
  num_init = 1L,
  init_fraction = 1,
  initializer = "kmeans++",
  compute_labels = TRUE,
  calc_wcss = FALSE,
  early_stop_iter = 10L,
  verbose = FALSE,
  CENTROIDS = NULL,
  tol = 1e-04
)
```

**Arguments**

- **data**: numeric or integer matrix-like object.
- **clusters**: the number of clusters.
- **batch_size**: the size of the mini batches.
- **max_iters**: the maximum number of clustering iterations.
- **num_init**: number of times the algorithm will be run with different centroid seeds.
- **init_fraction**: percentage of data to use for the initialization centroids (applies if initializer is kmeans++). Should be a float number between 0.0 and 1.0.
- **initializer**: the method of initialization. One of kmeans++ and random. See details for more information.
- **compute_labels**: logical indicating whether to compute the final cluster labels.
- **calc_wcss**: logical indicating whether the within-cluster sum of squares should be computed and returned (ignored if ‘compute_labels = FALSE’).
- **early_stop_iter**: continue that many iterations after calculation of the best within-cluster-sum-of-squared-error.
- **verbose**: logical indicating whether progress is printed on screen.
CENTROIDS an optional matrix of initial cluster centroids. The rows of the CENTROIDS matrix should be equal to the number of clusters and the columns should be equal to the columns of the data.

tol convergence tolerance.

Details

This function performs k-means clustering using mini batches. It was inspired by the implementation in https://github.com/mlampros/ClusterR.

The input matrix can be in any format supported by the ‘DelayedArray’ / ‘beachmat’ framework, including the matrix classes defined in the ‘Matrix’ package and the ‘HDFMatrix’ class.

There are two possible initializations.

kmeans++: kmeans++ initialization.

random: random selection of data rows as initial centroids.

Value

a list with the following attributes:

centroids: the final centroids;

WCSS_per_cluster (optional): the final per-cluster WCSS.

best_initialization: which initialization value led to the best WCSS solution;

iters_per_initialization: number of iterations per each initialization;

Clusters (optional): the final cluster labels.

References


Examples

data = matrix(1:30,nrow = 10)
mini_batch(data, 2, 10, 10)
**predict_mini_batch**

**Description**

Prediction function for mini-batch k-means applied to matrix-like objects.

**Usage**

```
predict_mini_batch(data, CENTROIDS)
```

**Arguments**

- **data**: matrix-like object containing numeric or integer data (observations in rows, variables in columns).
- **CENTROIDS**: a matrix of initial cluster centroids. The rows of the CENTROIDS matrix should be equal to the number of clusters and the columns should equal the columns of the data.

**Details**

This function takes the data and the output centroids and returns the clusters.

This implementation relies very heavily on the `MiniBatchKmeans` implementation. We provide the ability to work with other matrix-like objects other than base matrices (e.g. DelayedMatrix and HDF5Matrix) through the `beachmat` library.

**Value**

It returns a vector with the clusters.

**Author(s)**

Yuwei Ni

**Examples**

```
data(iris)
km = mini_batch(as.matrix(iris[,1:4]), clusters = 3,
                batch_size = 10, max_iters = 10)
clusters = predict_mini_batch(as.matrix(iris[,1:4]),
                              CENTROIDS = km$centroids)
```
**predict_mini_batch_r**  
*Compute labels for mini-batch k-means*

**Description**

Given a data matrix and a centroid matrix, it assigns each data point to the closest centroid, using block processing.

**Usage**

```r
predict_mini_batch_r(
  data,  
  centroids,  
  BPPARAM = BiocParallel::SerialParam(),  
  ...  
)
```

**Arguments**

- `data`: a matrix-like object with features in row and samples in columns.
- `centroids`: a matrix with the coordinates of the centroids.
- `BPPARAM`: for parallel computations. See the ‘BiocParallel’ package.
- `...`: passed to ‘blockApply’.

**Value**

A vector of cluster labels for each observation.

**Examples**

```r
data(iris)
kmc <- mini_batch(as.matrix(iris[,1:4]), clusters = 3,  
  batch_size = 10, max_iter = 100)
predict_mini_batch_r(t(as.matrix(iris[,1:4])), km$centroids)
```
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