Package ‘retrofit’

March 28, 2024

Title RETROFIT: Reference-free deconvolution of cell mixtures in spatial transcriptomics

Version 1.2.0

Description RETROFIT is a Bayesian non-negative matrix factorization framework to decompose cell type mixtures in ST data without using external single-cell expression references. RETROFIT outperforms existing reference-based methods in estimating cell type proportions and reconstructing gene expressions in simulations with varying spot size and sample heterogeneity, irrespective of the quality or availability of the single-cell reference. RETROFIT recapitulates known cell-type localization patterns in a Slide-seq dataset of mouse cerebellum without using any single-cell data.

biocViews Transcriptomics, Visualization, RNASeq, Bayesian, Spatial, Software, GeneExpression, DimensionReduction, FeatureExtraction, SingleCell

License GPL-3

Encoding UTF-8

LazyData FALSE

URL https://github.com/qunhualilab/retrofit

BugReports https://github.com/qunhualilab/retrofit/issues

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RoxygenNote 7.2.3

Depends R (>= 4.2), Rcpp

LinkingTo Rcpp

Suggests BiocStyle, knitr, rmarkdown, testthat, DescTools, ggplot2, corrplot, cowplot, grid, colorspace, png, reshape2, pals, RCurl

VignetteBuilder knitr

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annotateWithCorrelations

**Description**

Match cell types based on correlations with reference. `decomp_w` between matching algorithm.

**Usage**

```r
annotateWithCorrelations(sc_ref, K, decomp_w, decomp_h)
```

**Arguments**

- `sc_ref` A Matrix or Array with two dimensions (GeneExpressions, Cell types).
- `K` integer: The number of cell types to be selected
- `decomp_w` Matrix(GeneExpressions, Components): Decomposed w matrix
- `decomp_h` Matrix(Components, Spots): Decomposed h matrix
**Value**

A list of selected components, cells, and correlations

- **w**: Filtered 2d array with GeneExpressions, Cell types
- **h**: Filtered 2d array with Cell types, Spots
- **ranked_cells**: The list of cell names
- **ranked_correlations**: The list of correlations

**See Also**

papers reference

**Examples**

```r
data("testSimulationData")
K = 10
sc_ref = testSimulationData$sc_ref
W = testSimulationData$decompose$w
H = testSimulationData$decompose$h
result = retrofit::annotateWithCorrelations(sc_ref=sc_ref, K=K, decomp_w=W, decomp_h=H)
H_annotated = result$h
W_annotated = result$w
ranked_cells = result$ranked_cells
```

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**annotateWithMarkers**

**RETROFIT matching algorithm**

**Description**

Match cell types based on correlations with reference. decomp_w between matching algorithm description

**Usage**

```r
annotateWithMarkers(marker_ref, K, decomp_w, decomp_h)
```

**Arguments**

- **marker_ref**: Key-value list: A dictionary of key: cell type, value: GeneExpression list
- **K**: integer: The number of cell types to be selected
- **decomp_w**: Matrix(GeneExpressions, Components): Decomposed w matrix
- **decomp_h**: Matrix(Components, Spots): Decomposed h matrix
decompose

Value

A list of

• w
• h

See Also

papers reference

Examples

data("testSimulationData")
K = 10
marker_ref = testSimulationData$marker_ref
W = testSimulationData$decompose$w
H = testSimulationData$decompose$h
result = retrofit::annotateWithMarkers(marker_ref=marker_ref, K=K,
    decomp_w=W, decomp_h=H)
H_annotated = result$h
W_annotated = result$w
ranked_cells = result$ranked_cells

decompose

RETROFIT decomposition algorithm

Description

Receiving the input with 2d spatial transcriptomics matrix, the function returns factorized W, H, Theta. This function fulfills Structured Stochastic Variational Inference Algorithm for RETROFIT. Since exact Bayesian inference is infeasible and considering the large number of spots and genes, variational inference was adopted to approximately estimate the parameters in performant manner.

Usage

decompose(
  x,
  L = 16,
  iterations = 4000,
  init_param = NULL,
  lambda = 0.01,
  kappa = 0.5,
  verbose = FALSE
)
Arguments

- **x** matrix or array with dimension (GeneExpressions, Spots). This is the main spatial transcriptomics data.
- **L** integer (default:16) The number of components to be decomposed
- **iterations** integer (default:4000) The number of maximum iterations to be executed
- **init_param** list Vatirational initial parameters
- **lambda** double (default:0.01) Background expression profile control
- **kappa** double (default:0.5) Learning rate factor
- **verbose** boolean (default:FALSE)

Details

init_param specification

- **alpha_w_0** double (default:0.05)
- **beta_w_0** double (default:0.0001)
- **alpha_h_0** double (default:0.2)
- **beta_h_0** double (default:0.2)
- **alpha_th_0** double (default:1.25)
- **beta_th_0** double (default:10)
- **alpha_th_k** array (default:array with dim c(K))
- **beta_th_k** array (default:array with dim c(K)),
- **alpha_w_gk** array (default:array with dim c(G,K)),
- **beta_w_gk** array (default:array with dim c(G,K)),
- **alpha_h_ks** array (default:array with dim c(K,S)),
- **beta_h_ks** array (default:array with dim c(K,S))

Value

A list of decomposed vectors that contains

- **w**: 2d array with GeneExpressions, Components
- **h**: 2d array with Components, Spots
- **th**: an array with Components
- **durations**: (verbose) durations vector (unit: second)
- **relative_error**: (verbose) errors with pre-defined norm vector

See Also

papers reference
Examples

```r
data("testSimulationData")
x = testSimulationData$extra5_x
res = retrofit::decompose(x, L=16, iterations=10, verbose=TRUE)
W = res$w
H = res$h
TH = res$th
```

Description

The main algorithm

Usage

```r
retrofit(
  x,
  sc_ref = NULL,
  marker_ref = NULL,
  L = 16,
  K = 8,
  iterations = 4000,
  init_param = NULL,
  lambda = 0.01,
  kappa = 0.5,
  verbose = FALSE
)
```

Arguments

- **x**: A matrix or array with dimension (GeneExpressions, Spots). This is the main spatial transciptomics data.
- **sc_ref**: A matrix or array with two dimensions (GeneExpressions, Cell types).
- **marker_ref**: A list with (keys, values) = (cell types, an array of genes).
- **L**: integer (default:16) The number of components to be decomposed
- **K**: integer: The number of cell types to be selected
- **iterations**: integer (default:4000) The number of maximum iterations to be executed
- **init_param**: list Vatirational initial parameters
- **lambda**: double (default:0.01) Background expression profile control
- **kappa**: double (default:0.5) Learning rate factor
- **verbose**: boolean (default:FALSE)
Value

A list of decomposed vectors that contains

- decompose:
  - w: Decomposed 2d array with GeneExpressions, Components
  - h: Decomposed 2d array with Components, Spots
  - th: 1d array with Components

- annotateWithCorrelations:
  - w: Filtered 2d array with GeneExpressions, Cell types
  - h: Filtered2d array with Cell types, Spots

- annotateWithMarkers:
  - w: Filtered 2d array with GeneExpressions, Cell types
  - h: Filtered2d array with Cell types, Spots

See Also

papers reference

Examples

data("testSimulationData")
iterations = 10
L = 16
K = 8
x = testSimulationData$extra5_x
sc_ref = testSimulationData$sc_ref
res = retrofit::retrofit(x, sc_ref=sc_ref, L=L, K=K, iterations=iterations)
W = res$decompose$w
W_annotated = res$annotateWithCorrelations$w
ranked_cells = res$annotateWithCorrelations$ranked_cells

Description

A dataset with input and output of retrofit functions for reproducibility tests.

Usage

data(testSimulationData)

Format

Includes input x, references and results with large iterations
vignetteColonData

**Description**

A dataset supporting the colon vignette process

**Usage**

data(vignetteColonData)

**Format**

Includes colon scenario x, references, a large iterations results.

**Details**

- vignetteColonData

vignetteSimulationData

**Description**

A dataset supporting the simulation vignette process

**Usage**

data(vignetteSimulationData)

**Format**

Includes n10m3 scenario x, references, a large iterations results.

**Details**

- vignetteSimulationData
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