

# Package ‘divergence’

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**Title** Divergence: Functionality for assessing omics data by divergence with respect to a baseline

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**Author** Wikum Dinalankara <wdd4001@med.cornell.edu>, Luigi Marchionni <marchion@jhu.edu>, Qian Ke <qke1@jhu.edu>

**Maintainer**

Wikum Dinalankara <wdd4001@med.cornell.edu>, Luigi Marchionni <marchion@jhu.edu>

**Description** This package provides functionality for performing divergence analysis as presented in Dinalankara et al, ``Digitizing omics profiles by divergence from a baseline'', PANS 2018. This allows the user to simplify high dimensional omics data into a binary or ternary format which encapsulates how the data is divergent from a specified baseline group with the same univariate or multivariate features.

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**License** GPL-2

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|               |                                                               |
|---------------|---------------------------------------------------------------|
| breastTCGA_ER | <i>ER positive or negative status of breast tumor samples</i> |
|---------------|---------------------------------------------------------------|

---

### Description

A factor indicating whether 887 breast samples in breastTCGA\_Mat are ER positive or ER negative. The matched normals have empty values.

### Usage

```
breastTCGA_ER
```

### Format

A Factor of length 887 of levels Negative and Positive (with 111 missing values for the normals).

### Source

<https://cancergenome.nih.gov/>

---

|                  |                                                 |
|------------------|-------------------------------------------------|
| breastTCGA_Group | <i>Normal or Tumor status of breast samples</i> |
|------------------|-------------------------------------------------|

---

**Description**

A factor indicating whether 887 breast samples in breastTCGA\_Mat are tumor or matched normal.

**Usage**

breastTCGA\_Group

**Format**

A Factor of length 887 of levels NORMAL and TUMOR.

**Source**

<https://cancergenome.nih.gov/>

---

|                |                                                            |
|----------------|------------------------------------------------------------|
| breastTCGA_Mat | <i>Gene expression for 260 genes in 887 breast samples</i> |
|----------------|------------------------------------------------------------|

---

**Description**

A data matrix containing a subset of the TCGA breast cancer dataset, with the gene level expression estimates in log2 transcripts per million for 887 breast samples.

**Usage**

breastTCGA\_Mat

**Format**

A data matrix with 260 rows and 887 columns.

**Source**

<https://cancergenome.nih.gov/>



---

`computeMultivariateBinaryMatrix`*Compute the binary matrix with digitized divergence coding*

---

**Description**

Function for obtaining the binary form for a matrix for multivariate divergence of data given a baseline range

**Usage**

```
computeMultivariateBinaryMatrix(seMat, Baseline)
```

**Arguments**

|                       |                                                                                                                                                                           |
|-----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>seMat</code>    | SummarizedExperiment with assay to be digitized, in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form. |
| <code>Baseline</code> | A Baseline object; this corresponds to the output of <code>findMultivariateGammaW-ithSupport()</code> or <code>computeMultivariateSupport()</code>                        |

**Value**

A matrix with the same columns as `Mat`, with rows being the multivariate features, containing the binary form data.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = computeMultivariateSupport(seMat=seMat.base, FeatureSets=msigdb_Hallmarks)
dataMat = breastTCGA_Mat[, breastTCGA_Group != "NORMAL"]
seMat = SummarizedExperiment(assays=list(data=dataMat))
assays(seMat)$quantile = computeQuantileMatrix(seMat)
Mat.div = computeMultivariateBinaryMatrix(seMat=seMat, Baseline=baseline)
```

---

`computeMultivariateDigitization`*Perform binary digitization*

---

**Description**

Function for obtaining the digitized form, along with other relevant statistics and measures given a data matrix and a baseline matrix with multivariate features of interest

**Usage**

```
computeMultivariateDigitization(seMat, seMat.base, FeatureSets,
  computeQuantiles = TRUE, gamma = c(1:9/100, 1:9/10), beta = 0.95,
  alpha = 0.01, distance = "euclidean", verbose = TRUE,
  findGamma = TRUE, Groups = NULL, classes = NULL)
```

**Arguments**

|                  |                                                                                                                                                                                                                                                                         |
|------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat            | SummarizedExperiment with assay to be digitized, in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form.                                                                                               |
| seMat.base       | SummarizedExperiment with baseline assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature                                                                                                                                  |
| FeatureSets      | The multivariate features in list or matrix form. In list form, each list element should be a vector of individual features; in matrix form, it should be a binary matrix with rownames being individual features and column names being the names of the feature sets. |
| computeQuantiles | Apply quantile transformation to both data and baseline matrices (TRUE or FALSE; defaults to TRUE).                                                                                                                                                                     |
| gamma            | Range of gamma values to search through. By default gamma = 0.01, 0.02, ... 0.09, 0.1, 0.2, ..., 0.9.                                                                                                                                                                   |
| beta             | Parameter for eliminating outliers ( $0 < \beta \leq 1$ ). By default beta=0.95.                                                                                                                                                                                        |
| alpha            | Expected proportion of divergent features per sample to be estimated. The optimal gamma providing this level of divergence in the baseline data will be searched for.                                                                                                   |
| distance         | Type of distance to be calculated between points. Any type of distance that can be passed on to the dist function can be used (default 'euclidean').                                                                                                                    |
| verbose          | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                                                                                                                      |
| findGamma        | Logical indicating whether to search for optimal gamma values through the given gamma values (defaults to TRUE). If FALSE, the first value given in gamma will be used.                                                                                                 |
| Groups           | Factor indicating class association of samples                                                                                                                                                                                                                          |
| classes          | Vector of class labels                                                                                                                                                                                                                                                  |

**Value**

A list with elements: Mat.div: divergence coding of data matrix in binary form, of same dimensions at seMat baseMat.div: divergence coding of base matrix in binary form, of same column names at seMat.base, rows being multivariate features. div: data frame with the number of divergent features in each sample features.div: data frame with the divergent probability of each feature; divergence probability for each phenotype in included as well if 'Groups' and 'classes' inputs were provided. Baseline: a list containing a "Ranges" data frame with the baseline interval for each feature, and a "Support" binary matrix of the same dimensions as Mat indicating whether each sample was a support or a feature or not (1=support, 0=not in the support), gamma: selected gamma value alpha: the expected number of divergent features per sample computed over the baseline data matrix

**Examples**

```

baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
dataMat = breastTCGA_Mat[, breastTCGA_Group != "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
seMat = SummarizedExperiment(assays=list(data=dataMat))
div = computeMultivariateDigitization(
  seMat = seMat,
  seMat.base = seMat.base,
  FeatureSets = msigdb_Hallmarks
)

```

---

computeMultivariateSupport

*Estimate the baseline support*

---

**Description**

Function for computing the baseline support for multivariate features given gamma and beta parameters.

**Usage**

```

computeMultivariateSupport(seMat, FeatureSets, gamma = 0.1,
  beta = 0.95, distance = "euclidean", verbose = TRUE)

```

**Arguments**

|             |                                                                                                                                                                                                                                                                         |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat       | SummarizedExperiment with an assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form.                                                                                                             |
| FeatureSets | The multivariate features in list or matrix form. In list form, each list element should be a vector of individual features; in matrix form, it should be a binary matrix with rownames being individual features and column names being the names of the feature sets. |
| gamma       | Parameter for selecting radius around each support point ( $0 < \text{gamma} < 1$ ). By default $\text{gamma} = 0.1$ .                                                                                                                                                  |
| beta        | Parameter for eliminating outliers ( $0 < \text{beta} \leq 1$ ). By default $\text{beta} = 0.95$ .                                                                                                                                                                      |
| distance    | Type of distance to be calculated between points. Any type of distance that can be passed on to the dist function can be used (default 'euclidean').                                                                                                                    |
| verbose     | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                                                                                                                      |

**Value**

A list with elements: Support: a matrix indicating which samples were included in the support. Baseline\_list: a list where each element is the baseline of a multivariate feature. featureMat: the multivariate features in matrix form. alpha: the expected number of divergent multivariate features per sample. gamma: the gamma parameter used for baseline computation. distance: the type of distance used for baselien computation.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = computeMultivariateSupport(seMat=seMat.base, FeatureSets=msigdb_Hallmarks)
```

---

computeQuantileMatrix *Compute quantile transformations*

---

**Description**

Function for computing the quantile transformation for one or more samples supplied as columns of a matrix.

**Usage**

```
computeQuantileMatrix(seMat)
```

**Arguments**

seMat            A data matrix in SummarizedExperiment form, with each column corresponding to a sample and each row corresponding to a feature.

**Value**

A matrix of the same dimensions with the quantile data.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
```



---

 computeUnivariateDigitization

*Perform ternary digitization*


---

### Description

Function for obtaining the digitized form, along with other relevant statistics and measures given a data matrix and a baseline matrix

### Usage

```
computeUnivariateDigitization(seMat, seMat.base, computeQuantiles = TRUE,
  gamma = c(1:9/100, 1:9/10), beta = 0.95, alpha = 0.01,
  parallel = TRUE, verbose = TRUE, findGamma = TRUE, Groups = NULL,
  classes = NULL)
```

### Arguments

|                  |                                                                                                                                                                           |
|------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat            | SummarizedExperiment with assay to be digitized, in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form. |
| seMat.base       | SummarizedExperiment with baseline assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature                                    |
| computeQuantiles | Logical; apply quantile transformation to both data and baseline matrices (TRUE or FALSE; defaults to TRUE).                                                              |
| gamma            | Range of gamma values to search through. By default gamma = 0.01, 0.02, ... 0.09, 0.1, 0.2, ..., 0.9.                                                                     |
| beta             | Parameter for eliminating outliers ( $0 < \beta \leq 1$ ). By default beta=0.95.                                                                                          |
| alpha            | Expected proportion of divergent features per sample to be estimated. The optimal gamma providing this level of divergence in the baseline data will be searched for.     |
| parallel         | Logical indicating whether to compute features parallelly with mclapply on Unix based systems (defaults to TRUE, switched to FALSE if parallel package is not available). |
| verbose          | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                        |
| findGamma        | Logical indicating whether to search for optimal gamma values through the given gamma values (defaults to TRUE). If FALSE, the first value given in gamma will be used.   |
| Groups           | Factor indicating class association of samples (optional).                                                                                                                |
| classes          | Vector of class labels (optional).                                                                                                                                        |

**Value**

A list with elements: `Mat.div`: divergence coding of data matrix in ternary (-1, 0, 1) form, of same dimensions as `seMat`; `baseMat.div`: divergence coding of base matrix in ternary (-1, 0, 1) form, of same dimensions as `seMat`; `base`: data frame with the number of divergent features in each sample, including upper and lower divergence features; `div`: data frame with the divergent probability of each feature; divergence probability for each phenotype is included as well if 'Groups' and 'classes' inputs were provided. `Baseline`: a list containing a "Ranges" data frame with the baseline interval for each feature, and a "Support" binary matrix of the same dimensions as `Mat` indicating whether each sample was a support or a feature or not (1=support, 0=not in the support), `gamma`: selected gamma value, `alpha`: the expected number of divergent features per sample computed over the baseline data matrix, `optimal`: logical indicating whether the selected gamma value provided the necessary alpha requirement, `alpha_space`: a data frame with alpha values for each gamma searched

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
dataMat = breastTCGA_Mat[, breastTCGA_Group != "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
seMat = SummarizedExperiment(assays=list(data=dataMat))
div = computeUnivariateDigitization(
  seMat = seMat,
  seMat.base = seMat.base,
  parallel = TRUE
)
assays(seMat)$div = div$Mat.div
```

---

```
computeUnivariateSupport
```

*Estimate the baseline support*

---

**Description**

Function for computing the baseline support for univariate features given gamma and beta parameters.

**Usage**

```
computeUnivariateSupport(seMat, gamma = 0.1, beta = 0.95,
  parallel = TRUE, verbose = TRUE)
```

**Arguments**

|                    |                                                                                                                                                             |
|--------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <code>seMat</code> | SummarizedExperiment with an assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form. |
| <code>gamma</code> | Parameter for selecting radius around each support point ( $0 < \text{gamma} < 1$ ). By default <code>gamma = 0.1</code> .                                  |

|          |                                                                                                                                                                                        |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| beta     | Parameter for eliminating outliers ( $0 < \text{beta} \leq 1$ ). By default $\text{beta}=0.95$ .                                                                                       |
| parallel | Logical indicating whether to compute features parallelly with <code>mclapply</code> on Unix based systems (defaults to TRUE, switched to FALSE if parallel package is not available). |
| verbose  | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                                     |

**Value**

A list with elements "Ranges": data frame with the baseline interval for each feature, "Support": binary matrix of the same dimensions as `Mat` indicating whether each sample was a support for a feature or not (1=support, 0=not in the support), "gamma": gamma value, and "alpha": the expected number of divergent features per sample estimated over the samples.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = computeUnivariateSupport(seMat=seMat.base)
```

---

computeUnivariateTernaryMatrix

*Compute the ternary matrix with digitized divergence coding*

---

**Description**

Function for obtaining the ternary form for a matrix of data given a baseline range

**Usage**

```
computeUnivariateTernaryMatrix(seMat, Baseline)
```

**Arguments**

|          |                                                                                                                                                                                                                      |
|----------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat    | SummarizedExperiment with an assay in $[0, 1]$ , with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form.                                                       |
| Baseline | A list with a data frame element "Ranges" containing the baseline range of each features; this corresponds to the output of <code>findUnivariateGammaWithSupport()</code> or <code>computeUnivariateSupport()</code> |

**Value**

A matrix containing the ternary form data.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = computeUnivariateSupport(seMat=seMat.base)
dataMat = breastTCGA_Mat[, breastTCGA_Group != "NORMAL"]
seMat = SummarizedExperiment(assays=list(data=dataMat))
assays(seMat)$quantile = computeQuantileMatrix(seMat)
assays(seMat)$div = computeUnivariateTernaryMatrix(seMat=seMat, Baseline=baseline)
```

---

```
findMultivariateGammaWithSupport
```

*Find optimal gamma and corresponding support for list of feature sets*

---

**Description**

Function for searching through a range of gamma values for finding the smallest gamma and support that provides expected proportion of divergent features per sample less than or equal to alpha.

**Usage**

```
findMultivariateGammaWithSupport(seMat, FeatureSets, gamma = 1:9/10,
  beta = 0.95, alpha = 0.01, distance = "euclidean",
  verbose = TRUE)
```

**Arguments**

|             |                                                                                                                                                                                                                                                                         |
|-------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat       | SummarizedExperiment with an assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form.                                                                                                             |
| FeatureSets | The multivariate features in list or matrix form. In list form, each list element should be a vector of individual features; in matrix form, it should be a binary matrix with rownames being individual features and column names being the names of the feature sets. |
| gamma       | Range of gamma values to search through. By default gamma = {0.01, 0.02, ..., 0.09, 0.1, 0.2, ..., 0.9}.                                                                                                                                                                |
| beta        | Parameter for eliminating outliers ( $0 < \beta \leq 1$ ). By default beta=0.95.                                                                                                                                                                                        |
| alpha       | Expected proportion of divergent features per sample to be estimated over the samples in Mat. By default alpha = 0.01; i.e. search for the smallest gamma that provides 1% or less number of divergent features per sample.                                             |
| distance    | Type of distance to be calculated between points. Any type of distance that can be passed on to the dist function can be used (default 'euclidean').                                                                                                                    |
| verbose     | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                                                                                                                      |

**Value**

A list with elements: Support: a matrix indicating which samples were included in the support. Baseline: a list where each element is the baseline of a multivariate feature. featureMat: the multivariate features in matrix form. alpha: the expected number of divergent multivariate features per sample. gamma: the gamma parameter selected. distance: the type of distance used for baseliens computation. optimal: TRUE or FALSE indicating whether the alpha criteria was met alpha\_space: the alpha values corresponding to the gamma values searched through

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = findMultivariateGammaWithSupport(seMat=seMat.base, FeatureSets=msigdb_Hallmarks)
```

---

```
findUnivariateGammaWithSupport
```

*Search for optimal gamma and associated support*

---

**Description**

Function for searching through a range of gamma values for finding the smallest gamma that provides expected proportion of divergent features per sample less than or equal to alpha.

**Usage**

```
findUnivariateGammaWithSupport(seMat, gamma = c(1:9/100, 1:9/10),
  beta = 0.95, alpha = 0.01, parallel = TRUE, verbose = TRUE)
```

**Arguments**

|          |                                                                                                                                                                                                                             |
|----------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| seMat    | SummarizedExperiment with an assay in [0, 1], with each column corresponding to a sample and each row corresponding to a feature; usually in quantile form.                                                                 |
| gamma    | Range of gamma values to search through. By default gamma = {0.01, 0.02, ... 0.09, 0.1, 0.2, ..., 0.9}.                                                                                                                     |
| beta     | Parameter for eliminating outliers ( $0 < \beta \leq 1$ ). By default beta=0.95.                                                                                                                                            |
| alpha    | Expected proportion of divergent features per sample to be estimated over the samples in Mat. By default alpha = 0.01; i.e. search for the smallest gamma that provides 1% or less number of divergent features per sample. |
| parallel | Logical indicating whether to compute features parallelly with mclapply on Unix based systems (defaults to TRUE, switched to FALSE if parallel package is not available).                                                   |
| verbose  | Logical indicating whether to print status related messages during computation (defaults to TRUE).                                                                                                                          |

**Value**

A list with elements "Ranges": data frame with the baseline interval for each feature, "Support": binary matrix of the same dimensions as Mat indicating whether each sample was a support for a feature or not (1=support, 0=not in the support), "gamma": gamma value, and "alpha": the expected number of divergent features per sample estimated over the samples, "optimal": logical indicating whether the selected gamma value provided the necessary alpha requirement, and "alpha\_space": a data frame with alpha values for each gamma searched.

**Examples**

```
baseMat = breastTCGA_Mat[, breastTCGA_Group == "NORMAL"]
seMat.base = SummarizedExperiment(assays=list(data=baseMat))
assays(seMat.base)$quantile = computeQuantileMatrix(seMat.base)
baseline = findUnivariateGammaWithSupport(seMat=seMat.base)
```

---

msigdb\_Hallmarks

*Cancer Hallmark gene sets from the MSigDB collection*

---

**Description**

A subset of the cancer hallmarks functional gene sets from the MSigDB collection.

**Usage**

```
msigdb_Hallmarks
```

**Format**

A list of length 10, with the hallmark gene set name, each a character vector of gene symbols.

**Source**

<https://software.broadinstitute.org/gsea/msigdb/>

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