

Package ‘BatchQC’

May 5, 2024

Type Package

Title Batch Effects Quality Control Software

Version 2.0.0

Date 2024-04-02

Description Sequencing and microarray samples often are collected or processed in multiple batches or at different times. This often produces technical biases that can lead to incorrect results in the downstream analysis. BatchQC is a software tool that streamlines batch preprocessing and evaluation by providing interactive diagnostics, visualizations, and statistical analyses to explore the extent to which batch variation impacts the data. BatchQC diagnostics help determine whether batch adjustment needs to be done, and how correction should be applied before proceeding with a downstream analysis. Moreover, BatchQC interactively applies multiple common batch effect approaches to the data and the user can quickly see the benefits of each method. BatchQC is developed as a Shiny App. The output is organized into multiple tabs and each tab features an important part of the batch effect analysis and visualization of the data. The BatchQC interface has the following analysis groups: Summary, Differential Expression, Median Correlations, Heatmaps, Circular Dendrogram, PCA Analysis, Shape, ComBat and SVA.

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URL <https://github.com/wejlab/BatchQC>

BugReports <https://github.com/wejlab/BatchQC/issues>

Depends R (>= 4.3.0)

Imports data.table, DESeq2, dplyr, EBSeq, gg dendro, ggnewscale, ggplot2, limma, matrixStats, pheatmap, RColorBrewer, reader, reshape2, scan, shiny, stats, SummarizedExperiment, sva, tibble, tidyr, tidyverse, utils

Suggests BiocManager, BiocStyle, bladderbatch, dendextend, devtools, knitr, lintr, plotly, rmarkdown, shinythemes, spelling, testthat (>= 3.0.0)

VignetteBuilder knitr

biocViews BatchEffect, GraphAndNetwork, Microarray, Normalization,
PrincipalComponent, Sequencing, Software, Visualization,
QualityControl, RNASeq, Preprocessing, DifferentialExpression,
ImmunoOncology

Config/testthat/edition 3

Encoding UTF-8

Language en-US

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.1

git_url <https://git.bioconductor.org/packages/BatchQC>

git_branch RELEASE_3_19

git_last_commit 906d8d9

git_last_commit_date 2024-04-30

Repository Bioconductor 3.19

Date/Publication 2024-05-05

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| | |
|---------|------------------------------|
| BatchQC | <i>Run BatchQC shiny app</i> |
|---------|------------------------------|

Description

Run BatchQC shiny app

Usage

```
BatchQC(dev = FALSE)
```

Arguments

| | |
|-----|---------------------------------------|
| dev | Run the application in developer mode |
|-----|---------------------------------------|

Value

The shiny app will open

Examples

```
if(interactive()){  
  BatchQC()  
}
```

batchqc_explained_variation

Returns a list of explained variation by batch and condition combinations

Description

Returns a list of explained variation by batch and condition combinations

Usage

```
batchqc_explained_variation(se, batch, condition = NULL, assay_name)
```

Arguments

| | |
|------------|--|
| se | Summarized experiment object |
| batch | Batch covariate |
| condition | Condition covariate(s) of interest if desired, default is NULL |
| assay_name | Assay of choice |

Value

List of explained variation by batch and condition

Examples

```
library(scran)  
se <- mockSCE()  
batchqc_explained_variation <- BatchQC::batchqc_explained_variation(se,  
  batch = "Mutation_Status",  
  condition = "Treatment",  
  assay_name = "counts")  
  
batchqc_explained_variation
```

| | |
|---------------|--|
| batch_correct | <i>Batch Correct This function allows you to Add batch corrected count matrix to the SE object</i> |
|---------------|--|

Description

Batch Correct This function allows you to Add batch corrected count matrix to the SE object

Usage

```
batch_correct(se, method, assay_to_normalize, batch, group = NULL,
             covar, output_assay_name)
```

Arguments

| | |
|--------------------|-------------------------------------|
| se | SummarizedExperiment object |
| method | Normalization Method |
| assay_to_normalize | Which assay use to do normalization |
| batch | The batch |
| group | The group variable |
| covar | Covariate Matrix |
| output_assay_name | name of results assay |

Value

a summarized experiment object with normalized assay appended

Examples

```
library(scran)
se <- mockSCE()
se <- BatchQC::batch_correct(se, method = "ComBat-Seq",
                             assay_to_normalize = "counts",
                             batch = "Mutation_Status",
                             covar = "Treatment",
                             output_assay_name =
                               "ComBat_Seq_Corrected")
se <- BatchQC::batch_correct(se, method = "Combat",
                             assay_to_normalize = "counts",
                             batch = "Mutation_Status",
                             covar = "Treatment",
                             output_assay_name =
                               "Combat_Corrected")
se
```

| | |
|--------------|---|
| batch_design | <i>This function allows you to make a batch design matrix</i> |
|--------------|---|

Description

This function allows you to make a batch design matrix

Usage

```
batch_design(se, batch, covariate)
```

Arguments

| | |
|-----------|-----------------------|
| se | summarized experiment |
| batch | batch variable |
| covariate | biological covariate |

Value

design table

Examples

```
library(scran)
se <- mockSCE()
batch_design_tibble <- batch_design(se, batch = "Mutation_Status",
                                     covariate = "Treatment")

batch_design_tibble
```

| | |
|-----------------|---|
| batch_indicator | <i>Batch and Condition indicator for signature data</i> |
|-----------------|---|

Description

This dataset is from signature data captured when activating different growth pathway genes in human mammary epithelial cells (GEO accession: GSE73628). This data consists of three batches and ten different conditions corresponding to control and nine different pathways.

Usage

```
data(batch_indicator)
```

Format

A data frame with 89 rows and 2 variables:

batch batch

condition condition

| | |
|---------------------|--|
| bladder_data_upload | <i>Bladder data upload This function uploads the Bladder data set from the bladderbatch package. This dataset is from bladder cancer data with 22,283 different microarray gene expression data. It has 57 bladder samples with 3 metadata variables (batch, outcome and cancer). It contains 5 batches, 3 cancer types (cancer, biopsy, control), and 5 outcomes (Biopsy, mTCC, sTCC-CIS, sTCC+CIS, and Normal). Batch 1 contains only cancer, 2 has cancer and controls, 3 has only controls, 4 contains only biopsy, and 5 contains cancer and biopsy</i> |
|---------------------|--|

Description

Bladder data upload This function uploads the Bladder data set from the bladderbatch package. This dataset is from bladder cancer data with 22,283 different microarray gene expression data. It has 57 bladder samples with 3 metadata variables (batch, outcome and cancer). It contains 5 batches, 3 cancer types (cancer, biopsy, control), and 5 outcomes (Biopsy, mTCC, sTCC-CIS, sTCC+CIS, and Normal). Batch 1 contains only cancer, 2 has cancer and controls, 3 has only controls, 4 contains only biopsy, and 5 contains cancer and biopsy

Usage

```
bladder_data_upload()
```

Value

a SE object with counts data and metadata

Examples

```
library(bladderbatch)
se_object <- bladder_data_upload()
```

| | |
|-------------------|---|
| check_valid_input | <i>Helper function to check for valid input</i> |
|-------------------|---|

Description

Helper function to check for valid input

Usage

```
check_valid_input(se, batch, condition)
```

Arguments

| | |
|-----------|-----------|
| se | se object |
| batch | batch |
| condition | condition |

Value

True/False boolean; True if all input is valid, False if invalid

| | |
|---------------|----------------------|
| color_palette | <i>Color palette</i> |
|---------------|----------------------|

Description

This function creates the base color palette used in BatchQC

Usage

```
color_palette(n, first_hue = 25, last_hue = 360)
```

Arguments

| | |
|-----------|--|
| n | numeric object representing number of colors to be created |
| first_hue | numeric object to set the first hue value |
| last_hue | numeric object to set the final hue value |

Value

color_list list of colors generated

Examples

```
library(scrn)
n <- 100
color_list <- color_palette(n)
color_list
```

| | |
|-------------------|---|
| combat_correction | <i>Combat Correction This function applies combat correction to your summarized experiment object</i> |
|-------------------|---|

Description

Combat Correction This function applies combat correction to your summarized experiment object

Usage

```
combat_correction(se, assay_to_normalize, batch, covar, output_assay_name)
```

Arguments

| | |
|--------------------|------------------------------------|
| se | SummarizedExperiment object |
| assay_to_normalize | Assay that should be corrected |
| batch | The variable that represents batch |
| covar | Covariate Matrix |
| output_assay_name | name of results assay |

Value

SE object with an added combat corrected array

| | |
|-----------------------|---|
| combat_seq_correction | <i>Combat-Seq Correction This function applies combat-seq correction to your summarized experiment object</i> |
|-----------------------|---|

Description

Combat-Seq Correction This function applies combat-seq correction to your summarized experiment object

Usage

```
combat_seq_correction(se, assay_to_normalize, batch, group, covar,
output_assay_name)
```

Arguments

| | |
|--------------------|------------------------------------|
| se | SummarizedExperiment object |
| assay_to_normalize | Assay that should be corrected |
| batch | The variable that represents batch |
| group | The group variable |
| covar | Covariate Matrix |
| output_assay_name | name of results assay |

Value

SE object with an added combat-seq corrected array

| | |
|------------------|--|
| confound_metrics | <i>Combine std. Pearson correlation coefficient and Cramer's V</i> |
|------------------|--|

Description

Combine std. Pearson correlation coefficient and Cramer's V

Usage

```
confound_metrics(se, batch)
```

Arguments

| | |
|-------|-----------------------|
| se | summarized experiment |
| batch | batch variable |

Value

metrics of confounding

Examples

```
library(scran)
se <- mockSCE()
confound_table <- BatchQC::confound_metrics(se, batch = "Mutation_Status")
confound_table
```

`cor_props`*This function allows you to calculate correlation properties*

Description

This function allows you to calculate correlation properties

Usage

```
cor_props(bd)
```

Arguments

`bd` batch design

Value

correlation properties

Examples

```
library(scran)
se <- mockSCE()
batch_design_tibble <- batch_design(se, batch = "Mutation_Status",
                                   covariate = "Treatment")
correlation_property <- BatchQC::cor_props(batch_design_tibble)
correlation_property
```

`covariates_not_confounded`*Returns list of covariates not confounded by batch; helper function for explained variation and for populating shiny app condition options*

Description

Returns list of covariates not confounded by batch; helper function for explained variation and for populating shiny app condition options

Usage

```
covariates_not_confounded(se, batch)
```

Arguments

`se` Summarized experiment object
`batch` Batch variable

Value

List of explained variation by batch and condition

Examples

```
library(scran)
se <- mockSCE()
covariates_not_confounded <- BatchQC::covariates_not_confounded(se,
                                                                batch = "Mutation_Status")
covariates_not_confounded
```

cramers_v

This function allows you to calculate Cramer's V

Description

This function allows you to calculate Cramer's V

Usage

```
cramers_v(bd)
```

Arguments

bd batch design

Value

Cramer's V

Examples

```
library(scran)
se <- mockSCE()
batch_design_tibble <- batch_design(se, batch = "Mutation_Status",
                                    covariate = "Treatment")
cramers_v_result <- BatchQC::cramers_v(batch_design_tibble)
cramers_v_result
```

dendrogram_alpha_numeric_check
Dendrogram alpha or numeric checker

Description

This function checks if there is any numeric or strings for plotting legend

Usage

```
dendrogram_alpha_numeric_check(dendro_var)
```

Arguments

dendro_var column from dendrogram object representing category

Value

geom_label label for the legend of category variable

Examples

```
library(scran)
se <- mockSCE()
dendro_alpha_numeric_check <- dendrogram_alpha_numeric_check(
  dendro_var = "Treatment")
dendro_alpha_numeric_check
```

dendrogram_color_palette
Dendrogram color palette

Description

This function creates the color palette used in the dendrogram plotter

Usage

```
dendrogram_color_palette(col, dendrogram_info)
```

Arguments

col string object representing color of the label
dendrogram_info dendrogram_ends object

Value

annotation_color vector of colors corresponding to col variable

Examples

```
library(scran)
se <- mockSCE()
process_dendro <- BatchQC::process_dendrogram(se, "counts")
dendrogram_ends <- process_dendro$dendrogram_ends
col <- process_dendro$condition_var
dendro_colors <- dendrogram_color_palette(col = "Treatment",
                                         dendrogram_info = dendrogram_ends)
dendro_colors
```

dendrogram_plotter *Dendrogram Plot*

Description

This function creates a dendrogram plot

Usage

```
dendrogram_plotter(se, assay, batch_var, category_var)
```

Arguments

| | |
|--------------|--|
| se | SummarizedExperiment object |
| assay | assay to plot |
| batch_var | sample metadata column representing batch |
| category_var | sample metadata column representing category of interest |

Value

named list of dendrogram plots
dendrogram is a dendrogram ggplot
circular_dendrogram is a circular dendrogram ggplot


```

pval_summary(differential_expression)
pval_plotter(differential_expression)
assay_to_analyze = "counts")

```

| | |
|------------|---|
| EV_plotter | <i>This function allows you to plot explained variation</i> |
|------------|---|

Description

This function allows you to plot explained variation

Usage

```
EV_plotter(batchqc_ev)
```

Arguments

batchqc_ev table of explained variation from batchqc_explained_variation

Value

boxplot of explained variation

Examples

```

library(scrn)
se <- mockSCE()
se$Mutation_Status <- as.factor(se$Mutation_Status)
se$Treatment <- as.factor(se$Treatment)
expl_var_result <- batchqc_explained_variation(se, batch = "Mutation_Status",
                                             condition = "Treatment", assay_name = "counts")
EV_boxplot <- BatchQC::EV_plotter(expl_var_result[[1]])
EV_boxplot

```

| | |
|----------|--|
| EV_table | <i>EV Table Returns table with percent variation explained for specified number of genes</i> |
|----------|--|

Description

EV Table Returns table with percent variation explained for specified number of genes

Usage

```
EV_table(batchqc_ev)
```


Arguments

batchqc_ev explained variation results from batchqc_explained_variation

Value

List of explained variation by batch and condition

Examples

```
library(scran)
se <- mockSCE()
se$Mutation_Status <- as.factor(se$Mutation_Status)
se$Treatment <- as.factor(se$Treatment)
exp_var_result <- BatchQC::batchqc_explained_variation(se,
                                                    batch = "Mutation_Status",
                                                    condition = "Treatment",
                                                    assay_name = "counts")
EV_table <- BatchQC::EV_table(exp_var_result[[1]])

EV_table
```

get.res

Helper function to get residuals

Description

Helper function to get residuals

Usage

```
get.res(y, X)
```

Arguments

y assay
X model matrix design

Value

residuals

heatmap_num_to_char_converter

Heatmap numeric to character converter

Description

This function converts any found numerics to characters

Usage

```
heatmap_num_to_char_converter(ann_col)
```

Arguments

ann_col column data of heatmap

Value

ann_col modified column data of heatmap

Examples

```
library(scran)
se <- mockSCE()
col_info <- colData(se)
ann_col <- heatmap_num_to_char_converter(ann_col = col_info)
ann_col
```

heatmap_plotter

Heatmap Plotter

Description

This function allows you to plot a heatmap

Usage

```
heatmap_plotter(se, assay, nfeature, annotation_column, log_option)
```

Arguments

| | |
|-------------------|--|
| se | SummarizedExperiment |
| assay | normalized or corrected assay |
| nfeature | number of features to display |
| annotation_column | choose column |
| log_option | TRUE if data should be logged before plotting (recommended for sequencing counts), FALSE if data should not be logged (for instance, data is already logged) |

Value

heatmap plot

Examples

```
library(scran)
se <- mockSCE()
heatmaps <- BatchQC::heatmap_plotter(se,
                                     assay = "counts",
                                     nfeature = 15,
                                     annotation_column = c("Mutation_Status",
                                                           "Treatment"),
                                     log_option = FALSE)
correlation_heatmap <- heatmaps$correlation_heatmap
correlation_heatmap

heatmap <- heatmaps$topn_heatmap
heatmap
```

| | |
|--------------|---|
| normalize_SE | <i>This function allows you to add normalized count matrix to the SE object</i> |
|--------------|---|

Description

This function allows you to add normalized count matrix to the SE object

Usage

```
normalize_SE(se, method, log_bool, assay_to_normalize, output_assay_name)
```

Arguments

`se` SummarizedExperiment Object
`method` Normalization Method, either 'CPM' or 'DESeq' or 'none' for log only
`log_bool` True or False; True to log normalize the data set after normalization method
`assay_to_normalize` Which SE assay to do normalization on
`output_assay_name` name for the resulting normalized assay

Value

the original SE object with normalized assay appended

Examples

```
library(scran)
se <- mockSCE()
se_CPM_normalized <- BatchQC::normalize_SE(se, method = "CPM",
                                           log_bool = FALSE,
                                           assay_to_normalize = "counts",
                                           output_assay_name =
                                             "CPM_normalized_counts")
se_DESeq_normalized <- BatchQC::normalize_SE(se, method = "DESeq",
                                             log_bool = FALSE,
                                             assay_to_normalize = "counts",
                                             output_assay_name =
                                             "DESeq_normalized_counts")

se_CPM_normalized
se_DESeq_normalized
```

PCA_plotter

This function allows you to plot PCA

Description

This function allows you to plot PCA

Usage

```
PCA_plotter(se, nfeature, color, shape, assays, xaxisPC, yaxisPC,
            log_option = FALSE)
```

Arguments

| | |
|------------|--|
| se | SummarizedExperiment object |
| nfeature | number of features |
| color | choose a color |
| shape | choose a shape |
| assays | array of assay names from se |
| xaxisPC | the PC to plot as the x axis |
| yaxisPC | the PC to plot as the y axis |
| log_option | TRUE if data should be logged before plotting (recommended for sequencing counts), FALSE if data should not be logged (for instance, data is already logged); FALSE by default |

Value

List containing PCA info, PCA variance and PCA plot

Examples

```
library(scran)
se <- mockSCE()
se_object_ComBat_Seq <- BatchQC::batch_correct(se, method = "ComBat-Seq",
                                              assay_to_normalize = "counts",
                                              batch = "Mutation_Status",
                                              covar = "Treatment",
                                              output_assay_name =
                                                "ComBat_Seq_Corrected")
pca_plot <- BatchQC::PCA_plotter(se = se_object_ComBat_Seq,
                                nfeature = 2, color = "Mutation_Status",
                                shape = "Treatment",
                                assays = c("counts", "ComBat_Seq_Corrected"),
                                xaxisPC = 1, yaxisPC = 2, log_option = FALSE)

pca_plot$plot
pca_plot$var_explained
```

plot_data

This function formats the PCA plot using ggplot

Description

This function formats the PCA plot using ggplot

Usage

```
plot_data(pca_plot_data, color, shape, xaxisPC, yaxisPC)
```

Arguments

| | |
|---------------|--|
| pca_plot_data | Data for all assays to plot |
| color | variable that will be plotted as color |
| shape | variable that will be plotted as shape |
| xaxisPC | the PC to plot as the x axis |
| yaxisPC | the PC to plot as the y axis |

Value

PCA plot

| | |
|------------|------------------------------|
| preprocess | <i>Preprocess assay data</i> |
|------------|------------------------------|

Description

Preprocess assay data

Usage

```
preprocess(se, assay, nfeature, log_option)
```

Arguments

| | |
|------------|--|
| se | Summarized Experiment object |
| assay | Assay from SummarizedExperiment object |
| nfeature | Number of variable features to use |
| log_option | "True" if data should be logged, "False" otherwise |

Value

Returns processed data

process_dendrogram *Process Dendrogram*

Description

This function processes count data for dendrogram plotting

Usage

```
process_dendrogram(se, assay)
```

Arguments

| | |
|-------|-----------------------------|
| se | SummarizedExperiment object |
| assay | assay to plot |

Value

named list of dendrogram data
dendrogram_segments is data representing segments of the dendrogram
dendrogram_ends is data representing ends of the dendrogram

Examples

```
library(scran)
se <- mockSCE()
process_dendro <- BatchQC::process_dendrogram(se, "counts")
process_dendro
```

protein_data *Protein data with 39 protein expression levels*

Description

This data consists of two batches and two conditions corresponding to case and control. The columns are case/control samples, and the rows represent 39 different proteins.

Usage

```
data(protein_data)
```

Format

A data frame with 39 rows and 24 variables

| | |
|---------------------|--|
| protein_sample_info | <i>Batch and Condition indicator for protein expression data</i> |
|---------------------|--|

Description

This data consists of two batches and two conditions corresponding to case and control for the protein expression data

Usage

```
data(protein_sample_info)
```

Format

A data frame with 24 rows and 2 variables:

batch Batch Indicator

category Condition (Case vs Control) Indicator

| | |
|--------------|---|
| pval_plotter | <i>P-value Plotter This function allows you to plot p-values of explained variation</i> |
|--------------|---|

Description

P-value Plotter This function allows you to plot p-values of explained variation

Usage

```
pval_plotter(DE_results)
```

Arguments

DE_results Differential Expression analysis result (a named list of dataframes corresponding to each analysis completed with a "pvalue" column)

Value

boxplots of pvalues for each condition

Examples

```
library(scran)
se <- mockSCE()
differential_expression <- BatchQC::DE_analyze(se = se,
                                              method = "DESeq2",
                                              batch = "Treatment",
                                              conditions = c(
                                                "Mutation_Status"),
                                              assay_to_analyze = "counts")

pval_summary(differential_expression)
pval_plotter(differential_expression)
```

| | |
|--------------|---|
| pval_summary | Returns summary table for p-values of explained variation |
|--------------|---|

Description

Returns summary table for p-values of explained variation

Usage

```
pval_summary(res_list)
```

Arguments

res_list Differential Expression analysis result (a named list of dataframes corresponding to each analysis completed with a "pvalue" column)

Value

summary table for p-values of explained variation for each analysis

Examples

```
library(scran)
se <- mockSCE()
differential_expression <- BatchQC::DE_analyze(se = se,
                                              method = "DESeq2",
                                              batch = "Treatment",
                                              conditions = c(
                                                "Mutation_Status"),
                                              assay_to_analyze = "counts")

pval_summary(differential_expression)
```

| | |
|----------------|--|
| signature_data | <i>Signature data with 1600 gene expression levels</i> |
|----------------|--|

Description

This data consists of three batches and ten conditions. The columns are samples, and the rows represent 1600 different genes.

Usage

```
data(signature_data)
```

Format

A data frame with 1600 rows and 89 variables

| | |
|-----------------------|---|
| std_pearson_corr_coef | <i>Calculate a standardized Pearson correlation coefficient</i> |
|-----------------------|---|

Description

Calculate a standardized Pearson correlation coefficient

Usage

```
std_pearson_corr_coef(bd)
```

Arguments

| | |
|----|--------------|
| bd | batch design |
|----|--------------|

Value

standardized Pearson correlation coefficient

Examples

```
library(scran)
se <- mockSCE()
batch_design_tibble <- batch_design(se, batch = "Mutation_Status",
                                   covariate = "Treatment")
pearson_cor_result <- BatchQC::std_pearson_corr_coef(batch_design_tibble)
pearson_cor_result
```

summarized_experiment *This function creates a summarized experiment object from count and metadata files uploaded by the user*

Description

This function creates a summarized experiment object from count and metadata files uploaded by the user

Usage

```
summarized_experiment(counts, columndata)
```

Arguments

| | |
|------------|--------------------|
| counts | counts dataframe |
| columndata | metadata dataframe |

Value

a summarized experiment object

Examples

```
data(protein_data)
data(protein_sample_info)
se_object <- summarized_experiment(protein_data, protein_sample_info)
```

volcano_plot *Volcano plot*

Description

This function allows you to plot DE analysis results as a volcano plot

Usage

```
volcano_plot(DE_results, pslider = 0.05, fcslider)
```

Arguments

| | |
|------------|--|
| DE_results | a dataframe with the results of one of the DE Analysis; must include "log2FoldChange" and "pvalue" columns |
| pslider | Magnitude of significance value threshold, default is 0.05 |
| fcslider | Magnitude of expression change value threshold |

Value

A volcano plot of expression change and significance value data

Examples

```
library(scran)
se <- mockSCE()
differential_expression <- BatchQC::DE_analyze(se = se,
                                             method = "DESeq2",
                                             batch = "Treatment",
                                             conditions = c(
                                               "Mutation_Status",
                                               "Cell_Cycle"),
                                             assay_to_analyze = "counts")

value <- round((max(abs(
  differential_expression[[length(differential_expression)]][, 1]))
+ min(abs(
  differential_expression[[length(differential_expression)]][, 1])))) / 2)

volcano_plot(differential_expression[[1]], pslider = 0.05, fcslider = value)
```

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