Package: scBatchQC (via r-universe)

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Title Batch-Aware Cell Quality Control for Single-Cell RNA-seq

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Description scBatchQC provides a hierarchical empirical Bayes framework for quality control in multi-sample, multi-batch single-cell RNA-seq experiments. Unlike per-sample QC tools, scBatchQC jointly models QC metric distributions (library size, gene count, mitochondrial fraction) and doublet rates across batches, enabling calibrated cell-level QC calls that account for batch structure. The package operates natively on SingleCellExperiment objects and returns augmented colData with per-cell QC flags and batch-adjusted doublet scores.

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URL https://github.com/SubhadipJana1409/scBatchQC

BugReports https://github.com/SubhadipJana1409/scBatchQC/issues

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`scBatchQC-package` *scBatchQC: Batch-Aware Cell Quality Control for scRNA-seq*

Description

scBatchQC provides a hierarchical empirical Bayes framework for quality control (QC) in multi-sample, multi-batch single-cell RNA-sequencing (scRNA-seq) experiments.

Unlike per-sample QC tools such as `scuttle::isOutlier`, which apply a single global MAD threshold, `scBatchQC` jointly models QC metric distributions (library size, gene count, mitochondrial fraction) and doublet rates across batches. This prevents over-filtering of high-quality batches and under-filtering of low-quality ones — a common but underappreciated problem in multi-batch scRNA-seq workflows.

Main functions

`batchAwareQCMetrics` Compute per-cell QC metrics and flag outliers using batch-harmonized MAD thresholds.

`estimateBatchDoubletRate` Model expected doublet rates per batch as a function of cells loaded and protocol.

`harmonizeQCThresholds` Inspect and update harmonized thresholds at arbitrary MAD stringency.

`plotBatchQC` Visualize QC metric distributions per batch with threshold overlays.

Bioconductor data structures

All functions accept and return `SingleCellExperiment` objects. Results are stored as additional columns in `colData()`.

Author(s)

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References

Amezquita RA et al. (2020). Orchestrating single-cell analysis with Bioconductor. *Nature Methods*, 17, 137-145.

See Also

Useful links:

- https://github.com/SubhadipJana1409/scBatchQC
- Report bugs at https://github.com/SubhadipJana1409/scBatchQC/issues

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`batchAwareQCMetrics` *Batch-Aware QC Metric Computation*

Description

Computes per-cell quality control metrics and identifies outlier cells using a hierarchical empirical Bayes approach. Unlike `scuttle::isOutlier`, which applies a single global MAD threshold, `batchAwareQCMetrics` estimates batch-specific MAD scales and shrinks them toward a global prior, preventing over-filtering in high-quality batches and under-filtering in low-quality ones.

Usage

```
batchAwareQCMetrics(
  sce,
  batch = NULL,
  metrics = c("sum", "detected", "subsets_MT_percent"),
  nmads = 3,
  mt_pattern = "^MT-",
  shrink_strength = 0.5,
  BPPARAM = SerialParam()
)
```

Arguments

sce	A SingleCellExperiment object. Must have raw counts in assay(sce, "counts").
batch	A character(1) naming a column in colData(sce) that identifies batch membership. If NULL, falls back to standard per-dataset QC (equivalent to scuttle::isOutlier).
metrics	A character vector of QC metrics to evaluate. Supported: "sum" (library size), "detected" (genes detected), "subsets_MT_percent" (mitochondrial percentage). Default: all three.
nmads	A numeric(1) number of MADs to use as the outlier threshold. Default: 3.
mt_pattern	A character(1) regex used to identify mitochondrial genes. Default: "^MT-".
shrink_strength	A numeric(1) in [0, 1] controlling how much per-batch estimates are shrunk toward the global prior. 0 = no shrinkage (pure per-batch); 1 = full pooling. Default: 0.5 (empirical Bayes midpoint).
BPPARAM	A BiocParallelParam object controlling parallelisation. Default: SerialParam().

Details

For each QC metric m and batch b, the function estimates:

1. Per-batch median μ_b and MAD σ_b.
2. A shrinkage weight w_b based on batch cell count.
3. A global prior μ_0, σ_0 pooled across batches.
4. A harmonized threshold $\tau_b = \mu_b^* + nmads \times \sigma_b^*$ where μ_b^* and σ_b^* are the shrinkage estimates.

A cell is flagged as an outlier if any QC metric exceeds its batch-specific harmonized threshold.

Value

The input sce with the following additions to colData:

- scBatchQC_sum: library size (total UMI count).
- scBatchQC_detected: number of detected genes.
- scBatchQC_subsets_MT_percent: mitochondrial fraction.
- scBatchQC_outlier: logical flag; TRUE if the cell fails any QC threshold.
- scBatchQC_outlier_reason: character string naming which metric(s) caused the flag.

References

Lun ATL et al. (2016). A step-by-step workflow for low-level analysis of single-cell RNA sequencing data with Bioconductor. *F1000Research*, 5, 2122.

See Also

estimateBatchDoubletRate, harmonizeQCThresholds, plotBatchQC

Examples

```
library(SingleCellExperiment)

# Simulate a minimal SCE with two batches
set.seed(42)
counts <- matrix(rpois(2000, lambda = 5), nrow = 200, ncol = 100)
rownames(counts) <- paste0("Gene", seq_len(200))
rownames(counts)[1:10] <- paste0("MT-", seq_len(10))
colnames(counts) <- paste0("Cell", seq_len(100))

sce <- SingleCellExperiment(assays = list(counts = counts))
sce$batch <- rep(c("B1", "B2"), each = 50)

sce <- batchAwareQCMetrics(sce, batch = "batch")
table(sce$scBatchQC_outlier, sce$batch)
```

---

batchSummary *Accessor for batch summary in a BQCResult*

Description

Returns the per-batch summary `DataFrame`.

Usage

```
batchSummary(x, ...)

## S4 method for signature 'BQCResult'
batchSummary(x, ...)
```

Arguments

`x`	A `BQCResult` object.
`...`	Additional arguments (not used).

Value

A `DataFrame` of per-batch statistics.

Examples

```
library(S4Vectors)
obj <- BQCResult(
    qcFlags       = DataFrame(low_lib = c(FALSE, TRUE)),
    doubletScores = c(0.04, 0.06),
    batchSummary  = DataFrame(batch = "B1", doublet_rate_est = 0.04)
)
batchSummary(obj)
```

BQCResult *Constructor for BQCResult*

Description

Create a new `BQCResult` object.

Usage

```
BQCResult(qcFlags, doubletScores, batchSummary, params = list())
```

Arguments

`qcFlags`	A `DataFrame` of per-cell QC flags.
`doubletScores`	A numeric vector of doublet scores.
`batchSummary`	A `DataFrame` of per-batch statistics.
`params`	A list of analysis parameters.

Value

A `BQCResult` object.

Examples

```
library(S4Vectors)
qf <- DataFrame(low_lib = c(FALSE, TRUE, FALSE))
obj <- BQCResult(
    qcFlags       = qf,
    doubletScores = c(0.04, 0.06, 0.05),
    batchSummary  = DataFrame(batch = "B1", doublet_rate_est = 0.04)
)
obj
```

BQCResult-class *BQCResult: Batch-Aware QC Result Container*

Description

An S4 class to store the output of batch-aware quality control applied to a `SingleCellExperiment` object. Slots hold per-cell QC flags, batch-level doublet rate estimates, and harmonized QC thresholds for each batch.

Slots

`qcFlags` A `DataFrame` with per-cell logical QC flags, one row per cell and one column per QC metric.

`doubletScores` A `numeric` vector of batch-adjusted doublet probability scores, one per cell.

`batchSummary` A `DataFrame` with one row per batch summarising estimated doublet rate and harmonized thresholds.

`params` A `list` storing the parameters used in the analysis (batch variable name, NMAD multiplier, etc.).

`doubletScores` *Accessor for doublet scores in a BQCResult*

Description

Returns the per-cell doublet score vector.

Usage

```
doubletScores(x, ...)

## S4 method for signature 'BQCResult'
doubletScores(x, ...)
```

Arguments

`x`	A `BQCResult` object.
`...`	Additional arguments (not used).

Value

A `numeric` vector of doublet scores.

Examples

```
library(S4Vectors)
obj <- BQCResult(
    qcFlags       = DataFrame(low_lib = c(FALSE, TRUE)),
    doubletScores = c(0.04, 0.06),
    batchSummary  = DataFrame(batch = "B1", doublet_rate_est = 0.04)
)
doubletScores(obj)
```

`estimateBatchDoubletRate` *Estimate Per-Batch Doublet Rates*

Description

Estimates the expected doublet rate for each batch in a multi-sample `SingleCellExperiment` experiment. The doublet rate is modelled as a linear function of per-batch technical covariates (number of cells loaded, median library size, protocol type), enabling principled flagging of likely doublets across batches with heterogeneous capture efficiencies.

Usage

```
estimateBatchDoubletRate(
  sce,
  batch = NULL,
  cells_loaded = NULL,
  protocol = NULL,
  observed_doublets = NULL,
  return_sce = TRUE
)
```

Arguments

`sce`	A `SingleCellExperiment` object.
`batch`	A `character(1)` naming the batch column in `colData(sce)`.
`cells_loaded`	A named `numeric` vector with the number of cells loaded per batch (key = batch label, value = cell count loaded). If `NULL`, the observed cell count per batch is used as a proxy (underestimates doublet rate).
`protocol`	A named `character` vector mapping batch labels to protocol type (e.g. `"10x_v3"`, `"10x_v2"`, `"inDrop"`). Used to set the baseline k constant. Default: `NULL` (all batches assumed 10x v3).
`observed_doublets`	A `character(1)` naming a column in `colData(sce)` that contains externally computed doublet calls (`TRUE`/`FALSE`). When supplied, the model is calibrated against observed rates. Default: `NULL`.
`return_sce`	Logical. If `TRUE` (default), returns the input `sce` with `scBatchQC_doublet_rate` added to `colData`. If `FALSE`, returns a `DataFrame` of batch-level estimates.

Details

Doublet rates in droplet-based scRNA-seq follow approximately:

$$r_b \approx k \times N_b$$

where N_b is the number of cells loaded per batch and $k \approx 8 \times 10^{-6}$ for 10x Genomics Chromium.

estimateBatchDoubletRate allows k to vary by batch covariates (e.g. protocol, operator) by fitting a linear model on the log-transformed per-batch cell count. When external doublet simulations are not desired, this gives a lightweight alternative to full simulation-based tools like scDblFinder.

Optionally, if the user supplies observed doublet calls from an external tool in colData, the function will calibrate the rate model against those observations.

Value

If return_sce = TRUE: the input sce with a scBatchQC_doublet_rate column in colData giving the estimated doublet probability for each cell's batch. If return_sce = FALSE: a DataFrame with one row per batch and columns batch, n_cells_obs, cells_loaded, doublet_rate_est, protocol.

See Also

batchAwareQCMetrics, plotBatchQC

Examples

```
library(SingleCellExperiment)

set.seed(42)
counts <- matrix(rpois(2000, lambda = 5), nrow = 200, ncol = 100)
rownames(counts) <- paste0("Gene", seq_len(200))
colnames(counts) <- paste0("Cell", seq_len(100))

sce <- SingleCellExperiment(assays = list(counts = counts))
sce$batch <- rep(c("B1", "B2"), each = 50)

cells_loaded <- c(B1 = 5000, B2 = 8000)
sce <- estimateBatchDoubletRate(sce,
    batch = "batch",
    cells_loaded = cells_loaded
)
sce$scBatchQC_doublet_rate
```

---

harmonizeQCThresholds *Harmonize QC Thresholds Across Batches*

Description

Given a SingleCellExperiment that has already been processed by batchAwareQCMetrics, harmonizeQCThresholds returns the per-batch QC threshold table and optionally updates colData with revised flags at a user-specified stringency.

This is useful for interactive threshold exploration or for downstream reporting: instead of re-running the full QC pipeline, the user can sweep nmads and inspect how the number of flagged cells changes per batch.

Usage

```
harmonizeQCThresholds(
  sce,
  batch = NULL,
  nmads = 3,
  shrink_strength = 0.5,
  update_sce = FALSE
)
```

Arguments

sce	A SingleCellExperiment processed by batchAwareQCMetrics.
batch	A character(1) naming the batch column.
nmads	A numeric(1) MAD multiplier. Default: 3.
shrink_strength	A numeric(1) in [0, 1]. Default: 0.5.
update_sce	Logical. If TRUE, rewrites the scBatchQC_outlier and scBatchQC_outlier_reason columns in colData(sce) using the new thresholds. Default: FALSE.

Value

A list with components:

thresholds A named list of per-metric data.frames (rows = batches, columns = lower and upper).

n_flagged A DataFrame with one row per batch and one column per metric showing the number of cells that would be flagged at these thresholds.

sce The (possibly updated) sce, returned only when update_sce = TRUE.

See Also

batchAwareQCMetrics, estimateBatchDoubletRate, plotBatchQC

Examples

```
library(SingleCellExperiment)

set.seed(42)
counts <- matrix(rpois(2000, lambda = 5), nrow = 200, ncol = 100)
rownames(counts) <- paste0("Gene", seq_len(200))
rownames(counts)[1:10] <- paste0("MT-", seq_len(10))
colnames(counts) <- paste0("Cell", seq_len(100))

sce <- SingleCellExperiment(assays = list(counts = counts))
sce$batch <- rep(c("B1", "B2"), each = 50)
sce <- batchAwareQCMetrics(sce, batch = "batch")

# Explore with 2.5 MADs instead of default 3
result <- harmonizeQCThresholds(sce, batch = "batch", nmads = 2.5)
```

```
result$n_flagged
```

---

plotBatchQC *Visualize QC Metric Distributions Across Batches*

Description

Produces a panel of violin plots showing per-batch distributions of QC metrics, with harmonized threshold lines overlaid. Useful for inspecting whether batchAwareQCMetrics thresholds are sensible and for comparing batch quality visually.

Usage

```
plotBatchQC(
  sce,
  batch = NULL,
  metrics = NULL,
  show_thresholds = TRUE,
  nmads = 3,
  colour_by = "scBatchQC_outlier",
  point_size = 0.4,
  point_alpha = 0.4
)
```

Arguments

sce	A SingleCellExperiment processed by batchAwareQCMetrics.
batch	A character(1) naming the batch column in colData(sce).
metrics	A character vector of QC metric names to plot (without the "scBatchQC_" prefix). Default: all available.
show_thresholds	Logical. If TRUE, overlays the batch-specific harmonized upper thresholds as dashed horizontal lines. Default: TRUE.
nmads	Passed to harmonizeQCThresholds to recompute thresholds for display. Default: 3.
colour_by	A character(1) naming a colData column to colour cells by (e.g. "scBatchQC_outlier"). Default: "scBatchQC_outlier".
point_size	Numeric. Jitter point size. Default: 0.4.
point_alpha	Numeric. Jitter point alpha. Default: 0.4.

Value

A ggplot2 object. Can be modified with standard ggplot2 functions or saved with ggsave().

See Also

batchAwareQCMetrics, harmonizeQCThresholds

Examples

```
library(SingleCellExperiment)

set.seed(42)
counts <- matrix(rpois(2000, lambda = 5), nrow = 200, ncol = 100)
rownames(counts) <- paste0("Gene", seq_len(200))
rownames(counts)[1:10] <- paste0("MT-", seq_len(10))
colnames(counts) <- paste0("Cell", seq_len(100))

sce <- SingleCellExperiment(assays = list(counts = counts))
sce$batch <- rep(c("B1", "B2"), each = 50)
sce <- batchAwareQCMetrics(sce, batch = "batch")

plotBatchQC(sce, batch = "batch")
```

---

qcFlags *Accessor for QC flags in a BQCResult*

Description

Returns the per-cell QC flag DataFrame.

Usage

```
qcFlags(x, ...)

## S4 method for signature 'BQCResult'
qcFlags(x, ...)
```

Arguments

x	A BQCResult object.
...	Additional arguments (not used).

Value

A DataFrame of per-cell logical QC flags.

Examples

```
library(S4Vectors)
obj <- BQCResult(
    qcFlags       = DataFrame(low_lib = c(FALSE, TRUE)),
    doubletScores = c(0.04, 0.06),
    batchSummary  = DataFrame(batch = "B1", doublet_rate_est = 0.04)
)
qcFlags(obj)
```

`show,BQCResult-method` *Show method for BQCResult*

Description

Prints a compact summary of a `BQCResult` object.

Usage

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

Arguments

`object`	A `BQCResult` object.

Value

Invisibly returns `object`.

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