

Package: ExpoRiskR (via r-universe)

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Type Package

Title Exposure-Aware Multi-Omics Risk Modeling

Version 1.1.0

Description ExpoRiskR provides tools for exposure-aware multi-omics risk modeling in translational and environmental health studies. The package aligns sample identifiers across exposure and multi-omics blocks, performs lightweight preprocessing, and fits exposure-adjusted association models to build interpretable microbe–metabolite networks. It also computes simple exposure perturbation summaries and generates publication-ready visualizations. Workflows support both matrix-based inputs and SummarizedExperiment objects.

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URL <https://github.com/ppchaudhary/ExpoRiskR>

BugReports <https://github.com/ppchaudhary/ExpoRiskR/issues>

Imports stats, ggplot2, igraph, SummarizedExperiment, S4Vectors, utils

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align_omics	<i>Align exposures and multi-omics blocks by sample ID</i>
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Description

Ensures that microbiome, metabolome, exposures, and metadata all refer to the same set of samples in the same order. Sample IDs are taken from rownames of matrices/ data.frames, or from a column in meta if id_col is provided.

Usage

```
align_omics(
  microbiome,
  metabolome,
  exposures,
  meta,
  id_col = NULL,
  strict = TRUE
)
```

Arguments

microbiome	Matrix/data.frame of samples x microbes.
metabolome	Matrix/data.frame of samples x metabolites.
exposures	Matrix/data.frame of samples x exposures.
meta	data.frame of sample-level metadata (must include outcome later).
id_col	Optional column name in meta containing sample IDs. If NULL, rownames(meta) are used (if present).
strict	If TRUE, errors if any block has samples not found in others. If FALSE, intersects common samples and drops others.

Value

A list with aligned microbiome, metabolome, exposures, meta, and sample_id.

Examples

```
set.seed(4)
d <- generate_dummy_exporisk(n = 20, p_micro = 6, p_metab = 8, p_expo = 3)
aligned <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                      id_col = "sample_id", strict = TRUE)
names(aligned)
```

align_omics_se	<i>Align two SummarizedExperiment objects and extract exposures from colData</i>
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Description

Convenience wrapper to (i) align microbiome, metabolome, and exposures by sample ID and (ii) return two SummarizedExperiment objects (microbiome + metabolome) that share the same colData (meta + exposures). This is useful for Bioconductor-style workflows.

Inputs microbiome, metabolome, exposures are expected to be sample-by-feature matrices (or coercible to matrices). Sample IDs are taken from rownames when present; otherwise from meta[[id_col]].

Usage

```
align_omics_se(
  microbiome,
  metabolome,
  exposures,
  meta,
  id_col = "sample_id",
  strict = TRUE
)
```

Arguments

microbiome	Matrix/data.frame (samples x microbes).
metabolome	Matrix/data.frame (samples x metabolites).
exposures	Matrix/data.frame (samples x exposures).
meta	Data.frame with sample metadata including id_col.
id_col	Column name in meta holding sample IDs (default "sample_id").
strict	If TRUE, require that all blocks contain the same sample IDs; otherwise subset to the intersection (default TRUE).

Value

A list with:

- `se_microbiome`: SummarizedExperiment for microbiome (features x samples)
- `se_metabolome`: SummarizedExperiment for metabolome (features x samples)
- `exposures`: aligned numeric matrix (samples x exposures)
- `meta`: aligned meta data.frame
- `sample_ids`: character vector of aligned sample IDs

Examples

```
set.seed(7)
d <- generate_dummy_exporisk(n = 12, p_micro = 5, p_metab = 6, p_expo = 3)
out <- align_omics_se(
  d$microbiome, d$metabolome, d$exposures, d$meta,
  id_col = "sample_id", strict = TRUE
)
out$se_microbiome
out$se_metabolome
```

build_exposure_network

Build an exposure-adjusted microbe-metabolite association network

Description

For each (microbe, metabolite) pair, fits a linear model:

$$\text{metabolite} \sim \text{microbe} + \text{exposures} + \text{covariates}$$

and uses the microbe coefficient as the edge weight.

This is an MVP, interpretable approach suitable for Bioconductor submission.

Usage

```
build_exposure_network(
  X,
  Y,
  E,
  covar = NULL,
  fdr = 0.1,
  max_pairs = 5000,
  seed = NULL
)
```

Arguments

X	Numeric matrix (samples x microbes).
Y	Numeric matrix (samples x metabolites).
E	Numeric matrix (samples x exposures).
covar	Optional data.frame of sample-level covariates (rows = samples).
fdr	FDR threshold for keeping edges (BH adjusted p-value).
max_pairs	Max number of (microbe, metabolite) pairs to test (for speed). If NULL, tests all pairs (may be slow).
seed	Optional random seed used only when max_pairs is not NULL and sampling is required. If NULL, the current RNG state is used.

Value

A list with:

- edges: data.frame of significant edges (microbe, metabolite, weight, p_value, fdr)
- graph: igraph object (bipartite)
- meta: list of settings and counts

Examples

```
set.seed(1)
d <- generate_dummy_exporisk(n = 30, p_micro = 10, p_metab = 12, p_expo = 4)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
net <- build_exposure_network(pr$X, pr$Y, pr$E, fdr = 0.5, max_pairs = 120, seed = 1)
utils::head(net$edges)
```

exposure_perturbation_score

Score exposures by network perturbation (leave-one-exposure-out)

Description

Builds a reference network using all exposures, then for each exposure j builds a network leaving out exposure j, and computes a perturbation score based on differences in edge weights for a subset of tested pairs.

This is an MVP perturbation metric designed to be interpretable and fast enough for simulated/demo datasets.

Usage

```

exposure_perturbation_score(
  X,
  Y,
  E,
  covar = NULL,
  fdr = 0.2,
  max_pairs = 3000,
  seed = 1
)

```

Arguments

X	Microbiome matrix (samples x microbes).
Y	Metabolome matrix (samples x metabolites).
E	Exposures matrix (samples x exposures).
covar	Optional covariates data.frame.
fdr	FDR threshold passed to build_exposure_network().
max_pairs	Number of pairs to test per network build (speed control).
seed	Random seed.

Value

A data.frame with exposure, perturbation_score, n_edges_ref, n_edges_drop.

Examples

```

set.seed(2)
d <- generate_dummy_exporisk(n = 30, p_micro = 10, p_metab = 12, p_expo = 4)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
scores <- exposure_perturbation_score(pr$X, pr$Y, pr$E, fdr = 0.5, max_pairs = 120, seed = 1)
scores

```

```
generate_dummy_exporisk
```

Generate simulated exposure + multi-omics data with a binary outcome

Description

Creates a reproducible toy dataset for demonstrating ExpoRiskR workflows: exposures (E), microbiome-like positive features (X), metabolome-like positive features (Y), and a binary disease outcome.

If seed is provided, reproducibility is ensured locally without modifying the global RNG state.

Usage

```
generate_dummy_exporisk(
  n = 120,
  p_micro = 50,
  p_metab = 80,
  p_expo = 10,
  n_signal = 6,
  seed = NULL
)
```

Arguments

n	Number of samples.
p_micro	Number of microbiome features.
p_metab	Number of metabolomics features.
p_expo	Number of exposure variables.
n_signal	Number of truly associated features per block.
seed	Optional random seed for reproducible simulation.

Value

A list with matrices: microbiome, metabolome, exposures; and meta data.frame.

Examples

```
d <- generate_dummy_exporisk(n = 20, p_micro = 6, p_metab = 8, p_expo = 3, seed = 1)
str(d)
```

plot_exposure_network *Plot exposure-adjusted multi-omics network (bipartite)*

Description

Plots a bipartite igraph network returned by build_exposure_network(). Uses base igraph plotting (no extra dependencies).

Usage

```
plot_exposure_network(
  net,
  file = NULL,
  width = 10,
  height = 7,
  dpi = 300,
  layout = "layout_with_fr",
  max_label_nodes = 30
)
```

Arguments

net	A list returned by <code>build_exposure_network()</code> with elements <code>\$graph</code> and <code>\$edges</code> .
file	Optional output filename. If provided, saves a PNG (recommended).
width, height	Plot device size (in inches) when saving.
dpi	DPI when saving PNG.
layout	Layout function name passed to <code>igraph</code> . Default "layout_with_fr".
max_label_nodes	Max nodes to label (largest by degree). Default 30.

Value

Invisibly returns `net$graph`.

Examples

```
d <- generate_dummy_exporisk(seed = 1, n = 12, p_micro = 5, p_metab = 6, p_expo = 3)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
net <- build_exposure_network(pr$X, pr$Y, pr$E, fdr = 0.95, max_pairs = 120, seed = 1)
plot_exposure_network(net)
```

plot_exposure_ranking *Plot exposure perturbation ranking*

Description

Plot exposure perturbation ranking

Usage

```
plot_exposure_ranking(scores, top_n = 20)
```

Arguments

scores	A data.frame from <code>exposure_perturbation_score()</code> .
top_n	Show only top N exposures (default 20). Use NULL for all.

Value

A ggplot object.

Examples

```
d <- generate_dummy_exporisk(n = 30, p_micro = 10, p_metab = 12, p_expo = 4)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
scores <- exposure_perturbation_score(pr$X, pr$Y, pr$E,
                                     fdr = 0.5, max_pairs = 120, seed = 1)
plot_exposure_ranking(scores)
```

plot_feature_importance

Plot feature importance for exposures (logistic regression)

Description

Fits a logistic regression outcome ~ exposures and ranks exposures by the absolute standardized coefficient magnitude.

Usage

```
plot_feature_importance(E, outcome, top_n = 25)
```

Arguments

E	Numeric matrix (samples x exposures).
outcome	Binary vector (0/1), length = nrow(E).
top_n	Number of top exposures to show.

Value

A ggplot object.

Examples

```
d <- generate_dummy_exporisk(seed = 1, n = 20, p_micro = 6, p_metab = 8, p_expo = 4)
outcome <- d$meta$outcome
names(outcome) <- d$meta$sample_id
p <- plot_feature_importance(E = d$exposures, outcome = outcome, top_n = 10)
print(p)
```

plot_individual_risk_profile

Plot individual risk profile from exposure model

Description

Fits $\text{outcome} \sim \text{exposures}$ and shows per-exposure contribution for one sample based on standardized coefficients and standardized exposure values.

Usage

```
plot_individual_risk_profile(sample_id, E, outcome, top_n = 20)
```

Arguments

sample_id	Sample ID (must be in rownames(E)).
E	Numeric matrix (samples x exposures) with rownames.
outcome	Binary vector (0/1), named by sample IDs or same row order as E.
top_n	Number of top contributing exposures to display.

Value

A ggplot object.

Examples

```
d <- generate_dummy_exporisk(seed = 1, n = 20, p_micro = 6, p_metab = 8, p_expo = 4)
outcome <- d$meta$outcome
names(outcome) <- d$meta$sample_id
sid <- rownames(d$exposures)[1]
p <- plot_individual_risk_profile(sample_id = sid, E = d$exposures, outcome = outcome, top_n = 10)
print(p)
```

plot_network_stability

Plot network stability by bootstrap edge overlap

Description

Builds a reference network using all samples, then repeatedly bootstraps samples with replacement, rebuilds the network, and computes Jaccard overlap between edge sets.

Usage

```
plot_network_stability(  
  X,  
  Y,  
  E,  
  n_boot = 50,  
  fdr = 0.2,  
  max_pairs = 2000,  
  seed = NULL  
)
```

Arguments

X	Numeric matrix (samples x microbes).
Y	Numeric matrix (samples x metabolites).
E	Numeric matrix (samples x exposures).
n_boot	Number of bootstrap resamples.
fdr	FDR threshold passed to build_exposure_network().
max_pairs	Maximum pairs passed to build_exposure_network().
seed	Optional seed controlling bootstrap resampling only.

Value

A ggplot object.

Examples

```
d <- generate_dummy_exporisk(seed = 1, n = 20, p_micro = 8, p_metab = 10, p_expo = 4)  
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,  
  id_col = "sample_id", strict = TRUE)  
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)  
p <- plot_network_stability(pr$X, pr$Y, pr$E, n_boot = 2, fdr = 0.95, max_pairs = 120, seed = 1)  
print(p)
```

plot_risk_roc

Plot disease risk stratification ROC curves (MVP)

Description

Plot disease risk stratification ROC curves (MVP)

Usage

```
plot_risk_roc(X, Y, E, outcome, edges, top_edges = 200)
```

Arguments

X	Microbiome matrix (samples x features)
Y	Metabolome matrix (samples x features)
E	Exposures matrix (samples x features)
outcome	Binary vector (0/1)
edges	Network edges data.frame
top_edges	Number of strongest edges for network feature

Value

A ggplot object

Examples

```
d <- generate_dummy_exporisk(seed = 1, n = 25, p_micro = 8, p_metab = 10, p_expo = 4)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
net <- build_exposure_network(pr$X, pr$Y, pr$E, fdr = 0.95, max_pairs = 150, seed = 1)
outcome <- d$meta$outcome
names(outcome) <- d$meta$sample_id
p <- plot_risk_roc(pr$X, pr$Y, pr$E, outcome = outcome, edges = net$edges, top_edges = 30)
print(p)
```

```
prep_omics
```

Preprocess exposures and multi-omics blocks for modeling

Description

Lightweight preprocessing for MVP and Bioconductor-friendly workflows. Converts inputs to numeric matrices, checks sample alignment, optionally imputes missing values, applies log_{1p} transforms, and scales features.

Usage

```
prep_omics(
  microbiome,
  metabolome,
  exposures,
  log1p_micro = TRUE,
  log1p_metab = TRUE,
  z_expo = TRUE,
  scale_omics = TRUE,
  na_action = c("error", "impute")
)
```

Arguments

microbiome	Matrix/data.frame of samples x microbes.
metabolome	Matrix/data.frame of samples x metabolites.
exposures	Matrix/data.frame of samples x exposures.
log1p_micro	If TRUE (default), apply log1p to microbiome.
log1p_metab	If TRUE (default), apply log1p to metabolome.
z_expo	If TRUE (default), z-score exposures.
scale_omics	If TRUE (default), center/scale microbiome and metabolome features.
na_action	What to do with NA values: "error" (default) or "impute".

Value

A list with processed matrices: X, Y, E.

Examples

```
set.seed(1)
d <- generate_dummy_exporisk(n = 20, p_micro = 6, p_metab = 8, p_expo = 3)
al <- align_omics(d$microbiome, d$metabolome, d$exposures, d$meta,
                 id_col = "sample_id", strict = TRUE)
pr <- prep_omics(al$microbiome, al$metabolome, al$exposures)
str(pr)
```

```
prep_omics_se
```

Preprocess SummarizedExperiment-based omics blocks and exposures

Description

Preprocess SummarizedExperiment-based omics blocks and exposures

Usage

```
prep_omics_se(aligned, assay_micro = NULL, assay_metab = NULL, ...)
```

Arguments

aligned	Output from align_omics_se() or align_omics().
assay_micro	Assay name for microbiome SE (default: first assay).
assay_metab	Assay name for metabolome SE (default: first assay).
...	Passed to prep_omics().

Value

A list with preprocessed matrices: X, Y, E.

Examples

```
set.seed(8)
d <- generate_dummy_exporisk(n = 12, p_micro = 5, p_metab = 6, p_expo = 3)
aligned <- align_omics_se(d$microbiome, d$metabolome, d$exposures, d$meta,
  id_col = "sample_id", strict = TRUE)
se2 <- prep_omics_se(aligned)
se2
```

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