Package ‘qtbi’

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Title Quantum Toxic Burden Index

Version 0.1.2

Description Compute the Quantum Toxic Burden Index from multi-exposure panels using a fixed quantum-inspired entanglement encoder; method reference (2026) <doi:10.5281/zenodo.20476574>. Provides percentile encoding, optional potency-weighted readout, and synergy diagnostics for environmental mixture burden scores.

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URL `https://github.com/january-msemakweli/qtbi`, `https://doi.org/10.5281/zenodo.20476574`

BugReports `https://github.com/january-msemakweli/qtbi/issues`

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Contents

`build_statevector` *Build the n-qubit entanglement statevector for one subject*

Description

Build the n-qubit entanglement statevector for one subject

Usage

```
build_statevector(percentiles, synergy = 0.6)
```

Arguments

`percentiles`	Numeric vector of exposure percentiles in `[0, 1]`.
`synergy`	Synergy strength in `[0, 1]`.

Value

Complex statevector of length `2^n`.

`circuit_gate_schedule` *Gate schedule for circuit diagrams*

Description

Gate schedule for circuit diagrams

Usage

```
circuit_gate_schedule(n_exposures = 4L, n_metals = NULL)
```

Arguments

`n_exposures`	Number of exposures (qubits).
`n_metals`	Deprecated alias for `n_exposures`.

Value

List with gate schedule metadata.

`diagnose_qtbi` *Diagnose QTBI encoder behavior on processed data*

Description

Diagnose QTBI encoder behavior on processed data

Usage

```
diagnose_qtbi(
  data,
  synergy_grid = seq(0, 1, by = 0.05),
  synergy_ref = NULL,
  verbose = TRUE
)
```

Arguments

`data`	A `qtbi_data` object from `estimate_qtbi()`.
`synergy_grid`	Grid of synergy values for sensitivity curves.
`synergy_ref`	Reference synergy for summary statistics (defaults to the value used in `estimate_qtbi()`).
`verbose`	If `TRUE`, print a concise summary.

Value

A `qtbi_diagnosis` object (also printed when `verbose = TRUE`).

`estimate_qtbi` *Estimate QTBI and append scores to a data frame*

Description

Computes within-cohort exposure percentiles, runs the fixed entanglement encoder, and returns the input data with percentile and QTBI columns added.

Usage

```
estimate_qtbi(
  data,
  chemicals,
  synergy_strength = 0.6,
  qtbi_col = "qtbi",
  percentile_prefix = "pct_",
  exposure_names = NULL,
  pct_cols = NULL,
  reference_doses = NULL,
  reference_index = NULL
)
```

Arguments

`data`	A data frame containing exposure columns.
`chemicals`	Character vector of exposure column names.
`synergy_strength`	Synergy strength in `[0, 1]`.
`qtbi_col`	Name for the QTBI score column (default `"qtbi"`).
`percentile_prefix`	Prefix for percentile columns (default `"pct_"`).
`exposure_names`	Optional display names for plots (defaults to `chemicals`).
`pct_cols`	Optional percentile column names (same length as `chemicals`).
`reference_doses`	Optional named numeric vector of oral reference doses in mg/kg/day, with names matching `exposure_names` (or `chemicals` if `exposure_names` is omitted). The package derives potency weights as `reference_index` dose divided by each component dose, rescales them so their sum equals the number of exposures (keeping QTBI on the same $[0, n]$ scale as the unweighted index), and applies them at readout only.
`reference_index`	Name of the index chemical for potency ratios. Defaults to the first `exposure_names` entry (or first `chemicals` entry).

Value

A `qtbi_data` object (data frame) with QTBI and percentile columns.

Examples

```
df <- data.frame(
  Pb = c(1, 2, 3, 4),
  As = c(4, 3, 2, 1),
  Cd = c(2, 2, 3, 3),
  Hg = c(1, 3, 2, 4)
)
out <- estimate_qtbi(
  df,
  chemicals = c("Pb", "As", "Cd", "Hg"),
  synergy_strength = 0.6,
  reference_doses = c(Pb = 6.3e-4, As = 6.0e-5, Cd = 5.0e-4, Hg = 1.0e-4),
  reference_index = "Pb"
)
out$qtbi
```

`exposure_percentile` *Convert exposures to within-cohort percentiles*

Description

Convert exposures to within-cohort percentiles

Usage

```
exposure_percentile(x)
```

Arguments

`x`	Numeric exposure vector.

Value

Numeric percentiles in `(0, 1]`.

`is_qtbi_data` *Test for a qtbi_data object*

Description

Test for a qtbi_data object

Usage

```
is_qtbi_data(x)
```

Arguments

`x`	Object to test.

Value

`TRUE` if `x` inherits from `"qtbi_data"`.

`marginal_toxic_probs` *Marginal toxic probabilities from a QTBI statevector*

Description

Marginal toxic probabilities from a QTBI statevector

Usage

```
marginal_toxic_probs(state)
```

Arguments

`state`	Complex statevector from `build_statevector()`.

Value

Numeric vector of marginal toxic probabilities.

`normalize_potency_weights` *Rescale potency weights to match the unweighted QTBI scale*

Description

When potency weights are applied at readout, rescale them so their sum equals the number of exposures in the panel. This keeps weighted QTBI on the same $[0, n]$ scale as the unweighted sum of marginals, which aids comparison between weighted and unweighted analyses.

Usage

```
normalize_potency_weights(weights, target_sum = NULL)
```

Arguments

`weights`	Named numeric vector of raw potency ratios from `potency_weights_from_reference_doses()`.
`target_sum`	Target sum for the rescaled weights. Defaults to the number of exposures (`length(weights)`).

Value

Named numeric vector of rescaled weights aligned with `weights`.

`percentile_matrix` *Build percentile matrix from a data frame*

Description

Build percentile matrix from a data frame

Usage

```
percentile_matrix(data, chemicals)
```

Arguments

`data`	Data frame containing exposure columns.
`chemicals`	Character vector of column names.

Value

Numeric matrix with one percentile column per chemical.

`potency_weights_from_reference_doses` *Derive relative potency weights from reference doses*

Description

Computes outcome-independent weights as the ratio of the index chemical reference dose to each component reference dose:

$$w_i = \mathrm{RfD}_{\mathrm{index}}/\mathrm{RfD}_i$$

Usage

```
potency_weights_from_reference_doses(
  reference_doses,
  chemicals,
  reference_index = NULL
)
```

Arguments

`reference_doses`	Named numeric vector of oral reference doses in mg/kg/day, with one value per exposure in `chemicals`.
`chemicals`	Character vector of exposure identifiers in panel order. Names must match `names(reference_doses)`.
`reference_index`	Name of the index chemical. Defaults to the first entry in `chemicals`.

Details

Lower reference doses (more potent toxicants) receive larger weights.

Value

Named numeric vector of potency weights aligned with `chemicals`.

`qtbi_from_pcts` *Compute QTBI from percentile matrix*

Description

Compute QTBI from percentile matrix

Usage

```
qtbi_from_pcts(pct_mat, synergy = 0.6, weights = NULL)
```

Arguments

`pct_mat`	Numeric matrix of within-cohort percentiles (rows = subjects).
`synergy`	Synergy strength in `[0, 1]`.
`weights`	Optional named numeric potency weights aligned with columns.

Value

Numeric vector of QTBI scores.

`qtbi_from_state` *Compute QTBI from a statevector*

Description

Compute QTBI from a statevector

Usage

```
qtbi_from_state(state, weights = NULL)
```

Arguments

`state`	Complex statevector from `build_statevector()`.
`weights`	Optional named numeric potency weights aligned with qubits. When `NULL`, marginals are summed with equal weight.

Value

Scalar QTBI score (sum of marginal toxic probabilities).

`qtbi_from_vector` *Compute QTBI from one percentile vector*

Description

Compute QTBI from one percentile vector

Usage

```
qtbi_from_vector(pct_vec, synergy = 0.6, weights = NULL)
```

Arguments

`pct_vec`	Numeric vector of within-cohort percentiles.
`synergy`	Synergy strength in `[0, 1]`.
`weights`	Optional named numeric potency weights aligned with `pct_vec`.

Value

Scalar QTBI score.

`qtbi_help` *Package help index for qtbi*

Description

Prints a topic index for the main **qtbi** functions and optionally opens documentation for a specific topic. Use this when you want a guided entry point to the package; standard R help remains available via `?function_name` and `help(package = "qtbi")`.

Usage

```
qtbi_help(topic = NULL)
```

Arguments

`topic`	Optional character string naming a function or topic to open. If omitted, a summary index is printed.

Value

Invisibly returns `NULL`. When `topic` is supplied, the corresponding help page is opened as a side effect.

Examples

```
qtbi_help()
qtbi_help("estimate_qtbi")
```

`qtbi_meta` *Retrieve QTBI metadata stored on a processed data frame*

Description

Retrieve QTBI metadata stored on a processed data frame

Usage

```
qtbi_meta(data)
```

Arguments

`data`	A `qtbi_data` object from `estimate_qtbi()`.

Value

List with chemicals, synergy strength, and percentile column names.

`synergy_diagnostics` *Full circuit diagnostics for a cohort percentile matrix*

Description

Full circuit diagnostics for a cohort percentile matrix

Usage

```
synergy_diagnostics(
  pct_mat,
  synergy_grid = seq(0, 1, by = 0.05),
  synergy_ref = 0.6,
  exposure_names = NULL,
  metal_names = NULL,
  weights = NULL
)
```

Arguments

`pct_mat`	Numeric matrix of within-cohort percentiles (rows = subjects).
`synergy_grid`	Grid of synergy values in `[0, 1]`.
`synergy_ref`	Reference synergy for summary statistics.
`exposure_names`	Labels for exposures (columns of `pct_mat`).
`metal_names`	Deprecated alias for `exposure_names`.
`weights`	Optional potency weights aligned with columns of `pct_mat`.

Value

List with cohort_band, marginals, monotonicity, synergy_ref, sens_ref.

`synergy_sensitivity` *Synergy sensitivity on cohort median percentiles*

Description

Synergy sensitivity on cohort median percentiles

Usage

```
synergy_sensitivity(
  pct_mat,
  synergy_grid = seq(0, 1, by = 0.05),
  weights = NULL
)
```

Arguments

`pct_mat`	Numeric matrix of within-cohort percentiles.
`synergy_grid`	Grid of synergy values in `[0, 1]`.
`weights`	Optional potency weights aligned with columns of `pct_mat`.

Value

Data frame with synergy, qtbi, and additive_baseline columns.

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