

Package: qtbi (via r-universe)

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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](https://doi.org/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>,
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BugReports <https://github.com/january-msemakweli/qtbi/issues>

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build_statevector	<i>Build the n-qubit entanglement statevector for one subject</i>
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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:

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

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 $[\theta, 1]$.
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 $[\theta, 1]$.
weights	Optional named numeric potency weights aligned with pct_vec.

Value

Scalar QTBI score.

qtbi_help	<i>Package help index for qtbi</i>
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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.
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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	<i>Retrieve QTBI metadata stored on a processed data frame</i>
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Description

Retrieve QTBI metadata stored on a processed data frame

Usage

```
qtbi_meta(data)
```

Arguments

data	A <code>qtbi_data</code> object from <code>estimate_qtbi()</code> .
------	---

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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