

# Package ‘CompMix’

January 20, 2025

**Type** Package

**Title** A Comprehensive Toolkit for Environmental Mixtures Analysis  
(‘CompMix’)

**Version** 0.1.0

**Description** Quantitative characterization of the health impacts associated with exposure to chemical mixtures has received considerable attention in current environmental and epidemiological studies. ‘CompMix’ package allows practitioners to estimate the health impacts from exposure to chemical mixtures data through various statistical approaches, including Lasso, Elastic net, Bayesian kernel machine regression (BKMR), hierNet, Quantile g-computation, Weighted quantile sum (WQS) and Random forest. Hao W, Cathey A, Aung M, Boss J, Meeker J, Mukherjee B. (2024) ‘‘Statistical methods for chemical mixtures: a practitioners guide’’. <DOI:10.1101/2024.03.03.24303677>.

**License** GPL-3

**Imports** Matrix, mvtnorm, gglasso, higlasso, hierNet, glmnet,  
SuperLearner, bkmr, qqcomp, gWQS, pROC, randomForest, devtools

**Encoding** UTF-8

**RoxygenNote** 7.2.3

**NeedsCompilation** no

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**Repository** CRAN

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**Description**

A comprehensive toolkit for environmental mixtures analysis

**Usage**

```
Comp.Mix(
  y,
  x,
  z = NULL,
  y.type,
  test.pct = 0.5,
  var.select = NULL,
  interaction = NULL,
  interaction.exp.cov = NULL,
  covariates.forcein = NULL,
  bkmr.pip = 0.5,
  bkmr.iter = 500,
  formula = NULL,
  expnms = NULL,
  seed = 1234,
  verbose = TRUE
)
```

**Arguments**

y	A vector of either continuous or binary values to indicate the health outcome
x	A matrix of numeric values to indicate the chemical mixtures
z	A matrix of numeric values to indicate the covariates
y.type	A character value of either "continuous" or "binary"
test.pct	A numeric scalar between 0 and 1 to indicate the proportion allocated as test samples
var.select	A logical value to indicate whether to perform variable selection
interaction	A logical value (TRUE/FALSE) to indicate whether to include pairwise interaction terms between all the chemical mixtures x
interaction.exp.cov	A logical value (TRUE/FALSE) to indicate whether to include pairwise interaction terms between all the chemical mixtures x and covariates z. If interaction.exp.cov=TRUE, interaction=TURE or interaction=FALSE will be ignored
covariates.forcein	A logical value (TRUE/FALSE) to indicate whether to force in any covariates

<code>bkmr.pip</code>	A numeric scalar between 0 and 1 to indicate the cutoff for the posterior inclusion probability in BKMR
<code>bkmr.iter</code>	A positive integer to indicate the number of MCMC iterations for <code>bkmr</code>
<code>formula</code>	the formula for <code>qgcomp</code> and <code>wqs</code>
<code>expnms</code>	a vector of characters for names of exposure variables
<code>seed</code>	an integer value for seed
<code>verbose</code>	a logical value to show information

### Value

A list object which may contain up to 8 cases

**Case 1** variable selection on main effects for exposures and confounders

Each case may contain some of the following elements

**betaest** a numeric vector of coefficients for the exposures

**z\_betaest** a numeric vector of coefficients for the covariates

**sse** A positive scalar to indicate sum of squares error

**corr** A numeric scalar between -1 and 1 to indicate correlation coefficient

### Author(s)

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### Examples

```
dat <- lmi_simul_dat(n=1000,p=20,q=5,
  block_idx=c(1,1,2,2,3,1,1,1,1,1,2,2,2,2,3,3,3,3,3,3),
  within_rho=0.6,btw_rho=0.1,R2=0.2,
  effect_size=1,effect_size_i=1,
  cancel_effect = FALSE)
#Example 1: The users would like to perform variable selections
#on main effects of exposures and covariates, and outcome, exposures and
#covariates are entered. For any individual interactions that the users would
#like to include in the models, they can add those into the covariate z.
res_ex1 <- Comp.Mix(y.type="continuous",y=dat$y, x=dat$x, z=dat$z, test.pct=0.5,
  var.select = TRUE, interaction = FALSE, interaction.exp.cov = FALSE,
  covariates.forcein = FALSE,
  bkmr.pip=0.5, seed=2023)
```

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lmi\_simul\_dat

*Simulate data from linear model with interactions*


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### Description

Simulate data from linear model with interactions

### Usage

```
lmi_simul_dat(
  n,
  p,
  q,
  block_idx = c(1, 1, 2, 2, 3, 1, 1, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 3, 3),
  sigma2_x = 1,
  within_rho = 0.6,
  btw_rho = 0.2,
  R2 = 0.8,
  effect_size = 1,
  effect_size_i = 1,
  cancel_effect = TRUE
)
```

### Arguments

n	a positive integer to indicate sample size
p	a positive integer to specify the number of exposures
q	a positive integer to specify the number of non-zero effects
block_idx	a vector of positive integers to indicate the block IDs. The length of the vector is p.
sigma2_x	a positive numeric scalar for variance of the covariates
within_rho	a numeric scalar between 0 and 1 for the within block correlation
btw_rho	a numeric scalar between 0 and 1 for the between block correlation
R2	a numeric scalar for R-squared
effect_size	a numeric scalar for effect size for main effect
effect_size_i	a numeric scalar for effect size for interaction effect
cancel_effect	a logic value to indicate whether there is effect cancelation

### Value

a list object of the following

**x** covariate matrix of dimension n by p

**n** sample size

**p** number of covariates  
**sigma2\_x** variance  
**within\_rho** within block correlation  
**btw\_rho** between block correlation  
**block\_idx** block indices

**Author(s)**

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simul_x_block	<i>Simulate covariate matrix with block structure</i>
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**Description**

Simulate covariate matrix with block structure

**Usage**

```
simul_x_block(n, p, block_idx, sigma2_x = 1, within_rho = 0.6, btw_rho = 0.2)
```

**Arguments**

n	a positive integer to indicate sample size
p	a positive integer to specify the number of covariates
block_idx	a vector of positive integers to indicate the block IDs. The length of the vector is p.
sigma2_x	a positive numeric scalar for variance of the covariates
within_rho	a numeric scalar between 0 and 1 for the within block correlation
btw_rho	a numeric scalar between 0 and 1 for the between block correlation

**Value**

a list object of the following

**x** covariate matrix of dimension n by p  
**n** sample size  
**p** number of covariates  
**sigma2\_x** variance  
**within\_rho** within block correlation  
**btw\_rho** between block correlation  
**block\_idx** block indices

**Author(s)**

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**Examples**

```
dat <- simul_x_block(n = 1000, p = 10, block_idx = rep(1:4,length=10))
```

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