Package: MatrixCorrelation (via r-universe)

October 28, 2026

Encoding UTF-8

Type Package

Title Matrix Correlation Coefficients

Version 0.10.1

Date 2025-07-28

Description Computation and visualization of matrix correlation coefficients. The main method is the Similarity of Matrices Index, while various related measures like r1, r2, r3, r4, Yanai's GCD, RV, RV2, adjusted RV, Rozeboom's linear correlation and Coxhead's coefficient are included for comparison and flexibility.

URL https://github.com/khliland/MatrixCorrelation/

BugReports https://github.com/khliland/MatrixCorrelation/issues/

Depends R (>= 3.0.1)

Imports Rcpp, plotrix, pracma, progress, RSpectra

License GPL-2

LazyData TRUE

RoxygenNote 7.3.2

LinkingTo progress, Rcpp, RcppArmadillo

NeedsCompilation yes

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Repository https://cran.r-universe.dev

Date/Publication 2025-07-28 22:30:07 UTC

RemoteUrl https://github.com/cran/MatrixCorrelation

RemoteRef HEAD

RemoteSha 03aa9efc7d7a95e8cd729b7fd4f190717b8171be

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`allCorrelations` *All correlations*

Description

Compare all correlation measures in the package (or a subset)

Usage

```
allCorrelations(
  X1,
  X2,
  ncomp1,
  ncomp2,
  methods = c("SMI", "RV", "RV2", "RVadj", "PSI", "r1", "r2", "r3", "r4", "GCD"),
  digits = 3,
  plot = TRUE,
  xlab = "",
  ylab = "",
  ...
)
```

Arguments

`X1`	first `matrix` to be compared (`data.frames` are also accepted).
`X2`	second `matrix` to be compared (`data.frames` are also accepted).
`ncomp1`	maximum number of subspace components from the first `matrix`.
`ncomp2`	maximum number of subspace components from the second `matrix`.

`methods`	`character` vector containing a subset of the supported methods: "SMI", "RV", "RV2", "RVadj", "PSI", "r1", "r2", "r3", "r4", "GCD".
`digits`	number of digits for numerical output.
`plot`	logical indicating if plotting should be performed (default = TRUE).
`xlab`	optional x axis label.
`ylab`	optional y axis label.
`...`	additional arguments for `SMI` or `plot`.

Details

For each of the coefficients a single scalar is computed to describe the similarity between the two input matrices. Note that some methods requires setting one or two numbers of components.

Value

A single value measuring the similarity of two matrices.

Author(s)

Kristian Hovde Liland

References

SMI: Indahl, U.G.; Næs, T.; Liland, K.H.; 2018. A similarity index for comparing coupled matrices. Journal of Chemometrics; e3049.

RV: Robert, P.; Escoufier, Y. (1976). "A Unifying Tool for Linear Multivariate Statistical Methods: The RV-Coefficient". Applied Statistics 25 (3): 257-265.

RV2: Smilde, AK; Kiers, HA; Bijlsma, S; Rubingh, CM; van Erk, MJ (2009). "Matrix correlations for high-dimensional data: the modified RV-coefficient". Bioinformatics 25(3): 401-5.

Adjusted RV: Mayer, CD; Lorent, J; Horgan, GW. (2011). "Exploratory analysis of multiple omics datasets using the adjusted RV coefficient". Stat Appl Genet Mol Biol. 10(14).

PSI: Sibson, R; 1978. "Studies in the Robustness of Multidimensional Scaling: Procrustes Statistics". Journal of the Royal Statistical Society. Series B (Methodological), Vol. 40, No. 2, pp. 234-238.

Rozeboom: Rozeboom, WW; 1965. "Linear correlations between sets of variables". Psychometrika 30(1): 57-71.

Coxhead: Coxhead, P; 1974. "Measuring the releationship between two sets of variables". British Journal of Mathematical and Statistical Psychology 27: 205-212.

See Also

`SMI`, `RV` (RV2/RVadj), `r1` (r2/r3/r4/GCD).

Examples

```
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
usv <- svd(X1)
# Remove third principal component from X1 to produce X2
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

allCorrelations(X1,X2, ncomp1 = 5,ncomp2 = 5)
```

---

candy *Candy data*

Description

Measurements from sensory analysis (professional tasting) on a number of candy products obtained by sensory labs. The two labs and the associated data sets are parts of a larger study described in Tomic et al. (2010),

Usage

```
data(candy)
```

Format

Two matrices of dimension 18 x 6.

References

Tomic, O., Luciano, G., Nilsen, A., Hyldig, G., Lorensen, K., Næs, T. (2010). Analysing sensory panel performance in a proficiency test using the PanelCheck software. European Food Research and Technology. 230. 3, 497-511

---

cor.test_eq *Test for no correlation between paired sampes*

Description

Permutation test for squared Pearson correlation between to vectors of samples.

Usage

```
cor.test_eq(x, y, B = 10000)
```

Arguments

x	first vector to be compared (or two column matrix/data.frame).
y	second vector to be compared (ommit if included in x).
B	integer number of permutations, default = 10000.

Details

This is a convenience function combining SMI and significant for the special case of vector vs vector comparisons. The nullhypothesis is that the correlation between the vectors is +/-1, while significance signifies a deviance toward 0.

Value

A value indicating if the two input vectors are signficantly different.

Author(s)

Kristian Hovde Liland

References

Similarity of Matrices Index - Ulf Geir Indahl, Tormod Næs, Kristian Hovde Liland

See Also

plot.SMI (print.SMI/summary.SMI), RV (RV2/RVadj), r1 (r2/r3/r4/GCD), allCorrelations (matrix correlation comparison), PCAcv (cross-validated PCA).

Examples

```
a <- (1:5) + rnorm(5)
b <- (1:5) + rnorm(5)
cor.test_eq(a,b)
```

Coxhead *Coxhead's coefficient*

Description

Coxhead's coefficient

Usage

```
Coxhead(X1, X2, weighting = c("sqrt", "min"))
```

Arguments

X1	first matrix to be compared (data.frames are also accepted).
X2	second matrix to be compared (data.frames are also accepted).
weighting	string indicating if weighting should be sqrt(p*q) or min(p,q) (default = 'sqrt').

Value

A single value measuring the similarity of two matrices. For diagnostic purposes it is accompanied by an attribute "canonical.correlation".

References

Coxhead, P; 1974. "Measuring the releationship between two sets of variables". British Journal of Mathematical and Statistical Psychology 27: 205-212.

See Also

SMI, RV (RV2/RVadj), Rozeboom, r1 (r2/r3/r4/GCD).

Examples

```
X <- matrix(rnorm(100*13),nrow=100)
X1 <- X[, 1:5]  # Random normal
X2 <- X[, 6:12] # Random normal
X2[,1] <- X2[,1] + X[,5] # Overlap in one variable
Coxhead(X1, X2)
```

MatrixCorrelation *Similiarity of Matrices Coefficients*

Description

Computation and visualization of matrix correlation coefficients. The main method is the Similarity of Matrices Index, while various related measures like r1, r2, r3, r4, Yanai's GCD, RV, RV2, adjusted RV, Rozeboom's linear correlation and Coxhead's coefficient are included for comparison and flexibility.

Author(s)

Maintainer: Kristian Hovde Liland <kristian.liland@nmbu.no>

References

SMI: Indahl, U.G.; Næs, T.; Liland, K.H.; 2018. A similarity index for comparing coupled matrices. Journal of Chemometrics; e3049.

RV: Robert, P.; Escoufier, Y. (1976). "A Unifying Tool for Linear Multivariate Statistical Methods: The RV-Coefficient". Applied Statistics 25 (3): 257-265.

RV2: Smilde, AK; Kiers, HA; Bijlsma, S; Rubingh, CM; van Erk, MJ (2009). "Matrix correlations for high-dimensional data: the modified RV-coefficient". Bioinformatics 25(3): 401-5.

Adjusted RV: Mayer, CD; Lorent, J; Horgan, GW. (2011). "Exploratory analysis of multiple omics datasets using the adjusted RV coefficient". Stat Appl Genet Mol Biol. 10(14).

PSI: Sibson, R; 1978. "Studies in the Robustness of Multidimensional Scaling: Procrustes Statistics". Journal of the Royal Statistical Society. Series B (Methodological), Vol. 40, No. 2, pp. 234-238.

Rozeboom: Rozeboom, WW; 1965. "Linear correlations between sets of variables". Psychometrika 30(1): 57-71.

Coxhead: Coxhead, P; 1974. "Measuring the releationship between two sets of variables". British Journal of Mathematical and Statistical Psychology 27: 205-212.

See Also

`SMI`, `plot.SMI` (print.SMI/summary.SMI), `RV` (RV2/RVadj), `r1` (r2/r3/r4/GCD), `Rozeboom`, `Coxhead`, `allCorrelations` (matrix correlation comparison).

`PCAcv` *Principal Component Analysis cross-validation error*

Description

PRESS values for PCA as implemented by Eigenvector and described by Bro et al. (2008).

Usage

```
PCAcv(X, ncomp)
```

Arguments

`X`	`matrix` object to perform PCA on.
`ncomp`	`integer` number of components.

Details

For each number of components predicted residual sum of squares are calculated based on leave-one-out cross-validation. The implementation ensures no over-fitting or information bleeding.

Value

A vector of PRESS-values.

Author(s)

Kristian Hovde Liland

References

R. Bro, K. Kjeldahl, A.K. Smilde, H.A.L. Kiers, Cross-validation of component models: A critical look at current methods. Anal Bioanal Chem (2008) 390: 1241-1251.

See Also

`plot.SMI` (print.SMI/summary.SMI), `RV` (RV2/RVadj), `r1` (r2/r3/r4/GCD), `allCorrelations` (matrix correlation comparison).

Examples

```
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
PCAcv(X1,10)
```

`PCAimpute` *Principal Component Analysis based imputation*

Description

Imputation of missing data, NA, using Principal Component Analysis with iterative refitting and mean value updates. The chosen number of components and convergence parameters (iterations and tolerance) influence the precision of the imputation.

Usage

```
PCAimpute(X, ncomp, center = TRUE, max_iter = 20, tol = 10^-5)
```

Arguments

`X`	`matrix` object to perform PCA on.
`ncomp`	`integer` number of components.
`center`	`logical` indicating if centering (default) should be performed.
`max_iter`	`integer` number of iterations of PCA if sum of squared change in imputed values is above `tol`.
`tol`	`numeric` tolerance for sum of squared cange in imputed values.

Value

Final singular value decomposition, imputed `X` matrix and convergence metrics (sequence of sum of squared change and number of iterations).

Examples

```
X <- matrix(rnorm(12),3,4)
X[c(2,6,10)] <- NA
PCAimpute(X, 3)
```

`plot.SMI` *Result functions for the Similarity of Matrices Index (SMI)*

Description

Plotting, printing and summary functions for SMI, plus significance testing.

Usage

```
## S3 method for class 'SMI'
plot(
  x,
  y = NULL,
  x1lab = attr(x, "mat.names")[[1]],
  x2lab = attr(x, "mat.names")[[2]],
  main = "SMI",
  signif = 0.05,
  xlim = c(-(pq[1] + 1)/2, (pq[2] + 1)/2),
  ylim = c(0.5, (sum(pq) + 3)/2),
  B = 10000,
  cex = 1,
  cex.sym = 1,
  frame = NULL,
  frame.col = "red",
  frame.lwd = 2,
  replicates = NULL,
  ...
)

## S3 method for class 'SMI'
print(x, ...)

## S3 method for class 'SMI'
summary(object, ...)

is.signif(x, signif = 0.05, B = 10000, ...)
```

Arguments

x	object of class `SMI`.
y	not used.

x1lab	optional label for first matrix.
x2lab	optional label for second matrix.
main	optional heading (default = SMI).
signif	significance level for testing (default=0.05).
xlim	optional plotting limits.
ylim	optional plotting limits.
B	number of permutations (for significant, default=10000).
cex	optional text scaling (default = 1)
cex.sym	optional scaling for significance symbols (default = 1)
frame	two element integer vector indicating framed components.
frame.col	color for framed components.
frame.lwd	line width for framed components.
replicates	vector of replicates for significance testing.
...	additional arguments for plot.
object	object of class SMI.

Details

For plotting a diamonad plot is used. High SMI values are light and low SMI values are dark. If orthogonal projections have been used for calculating SMIs, significance symbols are included in the plot unless signif=NULL.

Value

plot silently returns NULL. print and summary return the printed matrix.

Author(s)

Kristian Hovde Liland

References

Similarity of Matrices Index - Ulf G. Indahl, Tormod Næs, Kristian Hovde Liland

See Also

SMI, PCAcv (cross-validated PCA).

Examples

```
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

smi <- SMI(X1,X2,5,5)
plot(smi, B = 1000) # default B = 10000
```

```
print(smi)
summary(smi)
is.signif(smi, B = 1000) # default B = 10000
```

PSI *Procrustes Similarity Index*

Description

An index based on the RV coefficient with Procrustes rotation.

Usage

```
PSI(X1, X2, center = TRUE)
```

Arguments

X1	first matrix to be compared (data.frames are also accepted).
X2	second matrix to be compared (data.frames are also accepted).
center	logical indicating if input matrices should be centered (default = TRUE).

Value

The Procrustes Similarity Index

References

Sibson, R; 1978. "Studies in the Robustness of Multidimensional Scaling: Procrustes Statistics". Journal of the Royal Statistical Society. Series B (Methodological), Vol. 40, No. 2, pp. 234-238.

Examples

```
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])
PSI(X1,X2)
```

r1 *Correlational Measures for Matrices*

Description

Matrix similarity as described by Ramsey et al. (1984).

Usage

```
r1(X1, X2, center = TRUE, impute = FALSE)

r2(
  X1,
  X2,
  center = TRUE,
  impute = FALSE,
  impute_par = list(max_iter = 20, tol = 10^-5)
)

r3(
  X1,
  X2,
  center = TRUE,
  impute = FALSE,
  impute_par = list(max_iter = 20, tol = 10^-5)
)

r4(
  X1,
  X2,
  center = TRUE,
  impute = FALSE,
  impute_par = list(max_iter = 20, tol = 10^-5)
)

GCD(
  X1,
  X2,
  ncomp1 = min(dim(X1)),
  ncomp2 = min(dim(X2)),
  center = TRUE,
  impute = FALSE,
  impute_par = list(max_iter = 20, tol = 10^-5)
)
```

Arguments

X1	first matrix to be compared (data.frames are also accepted).

X2	second matrix to be compared (data.frames are also accepted).
center	logical indicating if input matrices should be centered (default = TRUE).
impute	logical indicating if missing values are expected in X1 or X2.
impute_par	named list of imputation parameters in case of NAs in X1/X2.
ncomp1	(GCD) number of subspace components from the first matrix (default: full subspace).
ncomp2	(GCD) number of subspace components from the second matrix (default: full subspace).

Details

Details can be found in Ramsey's paper:

r1: inner product correlation

r2: orientation-independent inner product correlation

r3: spectra-independent inner product correlations (including orientation)

r4: Spectra-Independent inner product Correlations

GCD: Yanai's Generalized Coefficient of Determination (GCD) Measure. To reproduce the original GCD, use all components. When X1 and X2 are dummy variables, GCD is proportional with Pillai's criterion: tr(W^-1(B+W)).

Value

A single value measuring the similarity of two matrices.

Author(s)

Kristian Hovde Liland

References

Ramsay, JO; Berg, JT; Styan, GPH; 1984. "Matrix Correlation". Psychometrica 49(3): 403-423.

See Also

SMI, RV (RV2/RVadj), Rozeboom, Coxhead, allCorrelations (matrix correlation comparison), PCAcv (cross-validated PCA), PCAimpute (PCA based imputation).

Examples

```
X1  <- matrix(rnorm(100*300),100,300)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

r1(X1,X2)
r2(X1,X2)
r3(X1,X2)
r4(X1,X2)
```

```
GCD(X1,X2)
GCD(X1,X2, 5,5)

# Missing data
X1[c(1, 50, 400, 900)] <- NA
X2[c(10, 200, 450, 1200)] <- NA
r1(X1,X2, impute = TRUE)
r2(X1,X2, impute = TRUE)
r3(X1,X2, impute = TRUE)
r4(X1,X2, impute = TRUE)
GCD(X1,X2, impute = TRUE)
GCD(X1,X2, 5,5, impute = TRUE)
```

`Rozeboom` *Rozeboom's squared vector correlation*

Description

Rozeboom's squared vector correlation

Usage

```
Rozeboom(X1, X2)

sqveccor(X1, X2)
```

Arguments

`X1`	first `matrix` to be compared (`data.frames` are also accepted).
`X2`	second `matrix` to be compared (`data.frames` are also accepted).

Value

A single value measuring the similarity of two matrices. For diagnostic purposes it is accompanied by an attribute "canonical.correlation".

Author(s)

Korbinian Strimmer and Kristian Hovde Liland

References

Rozeboom, WW; 1965. "Linear correlations between sets of variables". Psychometrika 30(1): 57-71.

See Also

SMI, RV (RV2/RVadj), Coxhead, r1 (r2/r3/r4/GCD).

Examples

```
X <- matrix(rnorm(100*13),nrow=100)
X1 <- X[, 1:5]  # Random normal
X2 <- X[, 6:12] # Random normal
X2[,1] <- X2[,1] + X[,5] # Overlap in one variable
Rozeboom(X1, X2)
```

RV *RV coefficients*

Description

Three different RV coefficients: RV, RV2 and adusted RV.

Usage

```
RV(X1, X2, center = TRUE, impute = FALSE)

RV2(X1, X2, center = TRUE, impute = FALSE)

RVadjMaye(X1, X2, center = TRUE)

RVadjGhaziri(X1, X2, center = TRUE)

RVadj(X1, X2, version = c("Maye", "Ghaziri"), center = TRUE)
```

Arguments

X1	first matrix to be compared (data.frames are also accepted).
X2	second matrix to be compared (data.frames are also accepted).
center	logical indicating if input matrices should be centered (default = TRUE).
impute	logical indicating if missing values are expected in X1 or X2 (only for RV and RV2).
version	Which version of RV adjusted to apply: "Maye" (default) or "Ghaziri" RV adjusted is run using the RVadj function.

Details

For each of the four coefficients a single scalar is computed to describe the similarity between the two input matrices.

Value

A single value measuring the similarity of two matrices.

Author(s)

Kristian Hovde Liland, Benjamin Leutner (RV2)

References

RV: Robert, P.; Escoufier, Y. (1976). "A Unifying Tool for Linear Multivariate Statistical Methods: The RV-Coefficient". Applied Statistics 25 (3): 257-265.

RV2: Smilde, AK; Kiers, HA; Bijlsma, S; Rubingh, CM; van Erk, MJ (2009). "Matrix correlations for high-dimensional data: the modified RV-coefficient". Bioinformatics 25(3): 401-5.

Adjusted RV: Maye, CD; Lorent, J; Horgan, GW. (2011). "Exploratory analysis of multiple omics datasets using the adjusted RV coefficient". Stat Appl Genet Mol Biol. 10(14).

Adjusted RV: El Ghaziri, A; Qannari, E.M. (2015) "Measures of association between two datasets; Application to sensory data", Food Quality and Preference 40 (A): 116-124.

See Also

SMI, r1 (r2/r3/r4/GCD), Rozeboom, Coxhead, allCorrelations (matrix correlation comparison), PCAcv (cross-validated PCA), PCAimpute (PCA based imputation).

Examples

```
X1  <- matrix(rnorm(100*300),100,300)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

RV(X1,X2)
RV2(X1,X2)
RVadj(X1,X2)

# Missing data
X1[c(1, 50, 400, 900)] <- NA
X2[c(10, 200, 450, 1200)] <- NA
RV(X1,X2, impute = TRUE)
RV2(X1,X2, impute = TRUE)
```

---

significant *Significance estimation for Similarity of Matrices Index (SMI)*

Description

Permutation based hypothesis testing for SMI. The nullhypothesis is that a linear function of one matrix subspace is included in the subspace of another matrix.

Usage

```
significant(smi, B = 10000, replicates = NULL)
```

Arguments

smi	smi object returned by call to SMI.
B	integer number of permutations, default = 10000.
replicates	integer vector of replicates.

Details

For each combination of components significance is estimated by sampling from a null distribution of no similarity, i.e. when the rows of one matrix is permuted B times and corresponding SMI values are computed. If the vector replicates is included, replicates will be kept together through permutations.

Value

A matrix containing P-values for all combinations of components.

Author(s)

Kristian Hovde Liland

References

Similarity of Matrices Index - Ulf G. Indahl, Tormod Næs Kristian Hovde Liland

See Also

plot.SMI (print.SMI/summary.SMI), RV (RV2/RVadj), r1 (r2/r3/r4/GCD), allCorrelations (matrix correlation comparison).

Examples

```
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

(smi <- SMI(X1,X2,5,5))
significant(smi, B = 1000) # default B = 10000
```

SMI *Similarity of Matrices Index (SMI)*

Description

A similarity index for comparing coupled data matrices.

Usage

```
SMI(
  X1,
  X2,
  ncomp1 = Rank(X1) - 1,
  ncomp2 = Rank(X2) - 1,
  projection = "Orthogonal",
  Scores1 = NULL,
  Scores2 = NULL,
  impute = FALSE,
  impute_par = list(max_iter = 20, tol = 10^-5)
)
```

Arguments

X1	first matrix to be compared (data.frames are also accepted).
X2	second matrix to be compared (data.frames are also accepted).
ncomp1	maximum number of subspace components from the first matrix.
ncomp2	maximum number of subspace components from the second matrix.
projection	type of projection to apply, defaults to "Orthogonal", alternatively "Procrustes".
Scores1	user supplied score-matrix to replace singular value decomposition of first matrix.
Scores2	user supplied score-matrix to replace singular value decomposition of second matrix.
impute	logical for activation of PCA based imputation for X1/X2.
impute_par	named list of imputation parameters in case of NAs in X1/X2.

Details

A two-step process starts with extraction of stable subspaces using Principal Component Analysis or some other method yielding two orthonormal bases. These bases are compared using Orthogonal Projection (OP / ordinary least squares) or Procrustes Rotation (PR). The result is a similarity measure that can be adjusted to various data sets and contexts and which includes explorative plotting and permutation based testing of matrix subspace equality.

Value

A matrix containing all combinations of components. Its class is "SMI" associated with print, plot, summary methods.

Author(s)

Kristian Hovde Liland

References

Ulf Geir Indahl, Tormod Næs, Kristian Hovde Liland; 2018. A similarity index for comparing coupled matrices. Journal of Chemometrics; e3049.

See Also

plot.SMI (print.SMI/summary.SMI), RV (RV2/RVadj), r1 (r2/r3/r4/GCD), Rozeboom, Coxhead, allCorrelations (matrix correlation comparison), PCAcv (cross-validated PCA), PCAimpute (PCA based imputation).

Examples

```
# Simulation
X1  <- scale( matrix( rnorm(100*300), 100,300), scale = FALSE)
usv <- svd(X1)
X2  <- usv$u[,-3] %*% diag(usv$d[-3]) %*% t(usv$v[,-3])

(smi <- SMI(X1,X2,5,5))
plot(smi, B = 1000 ) # default B = 10000

# Sensory analysis
data(candy)
plot( SMI(candy$Panel1, candy$Panel2, 3,3, projection = "Procrustes"),
    frame = c(2,2), B = 1000, x1lab = "Panel1", x2lab = "Panel2" ) # default B = 10000

# Missing data (100 missing completely at random points each)
X1[sort(round(runif(100)*29999+1))] <- NA
X2[sort(round(runif(100)*29999+1))] <- NA
(smi <- SMI(X1,X2,5,5, impute = TRUE))
```

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