

# Package: rmi (via r-universe)

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**Title** Mutual Information Estimators

**Version** 0.1.1

**Author** Isaac Michaud [cre, aut]

**Maintainer** Isaac Michaud <ijmichau@ncsu.edu>

**Description** Provides mutual information estimators based on k-nearest neighbor estimators by A. Kraskov, et al. (2004) <[doi:10.1103/PhysRevE.69.066138](https://doi.org/10.1103/PhysRevE.69.066138)>, S. Gao, et al. (2015) <<http://proceedings.mlr.press/v38/gao15.pdf>> and local density estimators by W. Gao, et al. (2017) <[doi:10.1109/ISIT.2017.8006749](https://doi.org/10.1109/ISIT.2017.8006749)>.

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estimate_mse	<i>Estimate MSE of LNC Estimator</i>
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### Description

Computes the MSE of the Local Non-Uniformity Correct (LNC) KSG estimator for a given value of the tuning parameter alpha, dimension, neighborhood order, and sample size.

### Usage

```
estimate_mse(k = 5, alpha = 0, d = 2, rho = 0, N = 1000,
             M = 100, cluster = NULL)
```

### Arguments

k	Neighborhood order.
alpha	Non-uniformity threshold (see details).
d	Dimension.
rho	Reference correlation (see details).
N	Sample size.
M	Number of replications.
cluster	A parallel cluster object.

### Details

The parameter alpha controls the threshold for the application of the non-uniformity correction to a particular point's neighborhood. Roughly, alpha is the ratio of the PCA aligned neighborhood volume to the rectangular aligned neighborhood volume below which indicates non-uniformity and the correction is applied.

If  $\alpha < 0$  then a log scale is assumed; otherwise [0,1] scale is used.  $\alpha > 1$  are unacceptable values. A value of  $\alpha = 0$  forces no correction and LNC reverts to the KSG estimator.

The reference distribution that is assumed is a mean-zero multivariate normal distribution with a compound-symmetric covariance. The covariance matrix has a single correlation parameter supplied by rho.

**Examples**

```
estimate_mse(N = 100, M = 2)
```

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knn_mi	<i>kNN Mutual Information Estimators</i>
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**Description**

Computes mutual information based on the distribution of nearest neighborhood distances. Method available are KSG1 and KSG2 as described by Kraskov, et. al (2004) and the Local Non-Uniformity Corrected (LNC) KSG as described by Gao, et. al (2015). The LNC method is based on KSG2 but with PCA volume corrections to adjust for observed non-uniformity of the local neighborhood of each point in the sample.

**Usage**

```
knn_mi(data, splits, options)
```

**Arguments**

data	Matrix of sample observations, each row is an observation.
splits	A vector that describes which sets of columns in data to compute the mutual information between. For example, to compute mutual information between two variables use <code>splits = c(1,1)</code> . To compute <i>redundancy</i> among multiple random variables use <code>splits = rep(1, ncol(data))</code> . To compute the mutual information between two random vector list the dimensions of each vector.
options	A list that specifies the estimator and its necessary parameters (see details).

**Details**

Current available methods are LNC, KSG1 and KSG2.

For KSG1 use: `options = list(method = "KSG1", k = 5)`

For KSG2 use: `options = list(method = "KSG2", k = 5)`

For LNC use: `options = list(method = "LNC", k = 10, alpha = 0.65)`, order needed `k > ncol(data)`.

**Author**

Isaac Michaud, North Carolina State University, <ijmichau@ncsu.edu>

**References**

Gao, S., Ver Steeg G., & Galstyan A. (2015). Efficient estimation of mutual information for strongly dependent variables. *Artificial Intelligence and Statistics*: 277-286.

Kraskov, A., Stogbauer, H., & Grassberger, P. (2004). Estimating mutual information. *Physical review E* 69(6): 066138.

**Examples**

```

set.seed(123)
x <- rnorm(1000)
y <- x + rnorm(1000)
knn_mi(cbind(x,y),c(1,1),options = list(method = "KSG2", k = 6))

set.seed(123)
x <- rnorm(1000)
y <- 100*x + rnorm(1000)
knn_mi(cbind(x,y),c(1,1),options = list(method = "LNC", alpha = 0.65, k = 10))
#approximate analytic value of mutual information
-0.5*log(1-cor(x,y)^2)

z <- rnorm(1000)
#redundancy I(x;y;z) is approximately the same as I(x;y)
knn_mi(cbind(x,y,z),c(1,1,1),options = list(method = "LNC", alpha = c(0.5,0,0,0), k = 10))
#mutual information I((x,y);z) is approximately 0
knn_mi(cbind(x,y,z),c(2,1),options = list(method = "LNC", alpha = c(0.5,0.65,0), k = 10))

```

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lnn\_entropy

*Local Nearest Neighbor (LNN) Entropy Estimator*


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**Description**

Local Nearest Neighbor entropy estimator using Gaussian kernel and kNN selected bandwidth. Entropy is estimated by taking a Monte Carlo estimate using local kernel density estimate of the negative-log density.

**Usage**

```
lnn_entropy(data, k = 5, tr = 30, bw = NULL)
```

**Arguments**

data	Matrix of sample observations, each row is an observation.
k	Order of the local kNN bandwidth selection.
tr	Order of truncation (number of neighbors to include in entropy).
bw	Bandwidth (optional) manually fix bandwidth instead of using local kNN bandwidth selection.

**References**

Loader, C. (1999). Local regression and likelihood. Springer Science & Business Media.

Gao, W., Oh, S., & Viswanath, P. (2017). Density functional estimators with k-nearest neighbor bandwidths. IEEE International Symposium on Information Theory - Proceedings, 1, 1351–1355.

### Examples

```
set.seed(123)
x <- rnorm(1000)
print(lnn_entropy(x))
#analytic entropy
print(0.5*log(2*pi*exp(1)))
```

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lnn\_mi

*Local Nearest Neighbor (LNN) MI Estimator*

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### Description

Local Nearest Neighbor (LNN) mutual information estimator by Gao et al. 2017. This estimator uses the LNN entropy (`lnn_entropy`) estimator into the mutual information identity.

### Usage

```
lnn_mi(data, splits, k = 5, tr = 30)
```

### Arguments

<code>data</code>	Matrix of sample observations, each row is an observation.
<code>splits</code>	A vector that describes which sets of columns in data to compute the mutual information between. For example, to compute mutual information between two variables use <code>splits = c(1,1)</code> . To compute <i>redundancy</i> among multiple random variables use <code>splits = rep(1, ncol(data))</code> . To compute the mutual information between two random vector list the dimensions of each vector.
<code>k</code>	Order of the local kNN bandwidth selection.
<code>tr</code>	Order of truncation (number of neighbors to include in the local density estimation).

### References

Gao, W., Oh, S., & Viswanath, P. (2017). Density functional estimators with k-nearest neighbor bandwidths. IEEE International Symposium on Information Theory - Proceedings, 1, 1351–1355.

### Examples

```
set.seed(123)
x <- rnorm(1000)
y <- x + rnorm(1000)
lnn_mi(cbind(x,y), c(1,1))
```

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nearest_neighbors	<i>Compute Nearest Neighbors</i>
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## Description

Computes the nearest neighbor distances and indices of a sample using the infinite norm.

## Usage

```
nearest_neighbors(data, k)
```

## Arguments

data	Matrix of sample observations, each row is an observation.
k	Neighborhood order.

## Details

Nearest neighbors are computed using the brute-force method.

## Value

List of distances and indices of the k-nearest neighbors of each point in data.

## Examples

```
X <- cbind(1:10)
nearest_neighbors(X,3)

set.seed(123)
X <- cbind(runif(100),runif(100))
plot(X,pch=20)
points(X[3,1],X[3,2],col='blue',pch=19, cex=1.5)
nn <- nearest_neighbors(X,5)
a = X[nn$nn_inds[3,-1],1]
b = X[nn$nn_inds[3,-1],2]
points(a,b,col='red',pch=19, cex=1.5)
```

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optimize_mse	<i>Optimize MSE of LNC Estimator</i>
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## Description

Gaussian process (GP) optimization is used to minimize the MSE of the LNC estimator with respect to the non-uniformity threshold parameter  $\alpha$ . A normal distribution with compound-symmetric covariance is used as a reference distribution to optimize the MSE of LNC with respect to.

## Usage

```
optimize_mse(rho, N, M, d, k, lower = -10, upper = -1e-10,  
            num_iter = 10, init_size = 20, cluster = NULL, verbose = TRUE)
```

## Arguments

rho	Reference correlation.
N	Sample size.
M	Number of replications.
d	Dimension.
k	Neighborhood order.
lower	Lower bound for optimization.
upper	Upper bound for optimization.
num_iter	Number of iterations of GP optimization.
init_size	Number of initial evaluation to estimating GP.
cluster	A parallel cluster object.
verbose	If TRUE then print runtime diagnostic output.

## Details

The package `tgp` is used to fit a treed-GP to the MSE estimates of LNC. A treed-GP is used because the MSE of LNC with respect to  $\alpha$  exhibits clear non-stationarity. A treed-GP is able to identify the function's different correlation lengths which improves optimization.

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rmi

*Mutual Information Estimators*

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### **Description**

The rmi package offers a collection of mutual information estimators based on k-Nearest Neighbor and local density estimators. Currently, rmi provides the Kraskov et al. algorithm (KSG) 1 and 2, Local Non-uniformity Corrected (LNC) KSG, and the Local Nearest Neighbor (LNN) estimator. More estimators and examples will be incorporated in the future.

### **References**

- Gao, S., Ver Steeg G., & Galstyan A. (2015). Efficient estimation of mutual information for strongly dependent variables. *Artificial Intelligence and Statistics*: 277-286.
- Gao, W., Oh, S., & Viswanath, P. (2017). Density functional estimators with k-nearest neighbor bandwidths. *IEEE International Symposium on Information Theory - Proceedings*, 1, 1351–1355.
- Kraskov, A., Stogbauer, H., & Grassberger, P. (2004). Estimating mutual information. *Physical review E* 69(6): 066138.

### **Author(s)**

Isaac Michaud



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