Package ‘tensorEVD’

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Title A Fast Algorithm to Factorize High-Dimensional Tensor Product Matrices
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Description Here we provide tools for the computation and factorization of high-dimensional tensor products that are formed by smaller matrices. The methods are based on properties of Kronecker products (Searle 1982, p. 265, ISBN-10: 0470009616). We evaluated this methodology by benchmark testing and illustrated its use in Gaussian Linear Models (Lopez-Cruz et al., 2024) <doi:10.1093/g3journal/jkae001>.

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Hadamard product

Description
Computes the Hadamard product between two matrices.

Usage

Hadamard(A, B, IDrowA, IDrowB,
    IDcolA = NULL, IDcolB = NULL,
    make.dimnames = FALSE,
    drop = TRUE, inplace = FALSE)

Arguments
A (numeric) Left numeric matrix
B (numeric) Right numeric matrix
IDrowA (integer/character) Vector of length \( m \) with either indices or row names mapping from rows of \( A \) into the resulting hadamard product. If 'missing', it is assumed to be equal to 1,...,\( nrow(A) \)
IDrowB (integer/character) Vector of length \( m \) with either indices or row names mapping from rows of \( B \) into the resulting hadamard product. If 'missing', it is assumed to be equal to 1,...,\( nrow(B) \)
IDcolA (integer/character) (Optional) Similar to IDrowA, vector of length \( n \) for columns. If NULL, it is assumed to be equal to IDrowA if \( m = n \)
IDcolB (integer/character) (Optional) Similar to IDrowB, vector of length \( n \) for columns. If NULL, it is assumed to be equal to IDrowB if \( m = n \)
drop Either TRUE or FALSE to whether return a uni-dimensional vector when output is a matrix with either 1 row or 1 column as per the rows and cols arguments
make.dimnames TRUE or FALSE to whether add rownames and colnames attributes to the output
inplace TRUE or FALSE to whether operate directly on one input matrix (\( A \) or \( B \)) when this is used as is (i.e., is not indexed; therefore, needs to be of appropriate dimensions) in the Hadamard. When TRUE the output will be overwritten on the same address occupied by the non-indexed matrix. Default inplace=FALSE

Details
Computes the \( m \times n \) Hadamard product (aka element-wise or entry-wise product) matrix between matrices \( \mathbf{A} \) and \( \mathbf{B} \),

\[
(R_1 \mathbf{A} C_1') \odot (R_2 \mathbf{B} C_2')
\]
where \( R_1 \) and \( R_2 \) are incidence matrices mapping from rows of the resulting Hadamard to rows of \( A \) and \( B \), respectively; and \( C_1 \) and \( C_2 \) are incidence matrices mapping from columns of the resulting Hadamard to columns of \( A \) and \( B \), respectively.

Matrix \( R_1 AC'_1 \) can be obtained by matrix indexing as \( A[\text{IDrowA}, \text{IDcolA}] \), where \( \text{IDrowA} \) and \( \text{IDcolA} \) are integer vectors whose entries are, respectively, the row and column number of \( A \) that are mapped at each row of \( R_1 \) and \( C_1 \), respectively. Likewise, matrix \( R_2 BC'_2 \) can be obtained as \( B[\text{IDrowB}, \text{IDcolB}] \), where \( \text{IDrowB} \) and \( \text{IDcolB} \) are integer vectors whose entries are, respectively, the row and column number of \( B \) that are mapped at each row of \( R_2 \) and \( C_2 \), respectively. Therefore, the Hadamard product can be obtained directly as

\[
A[\text{IDrowA}, \text{IDcolA}]*B[\text{IDrowB}, \text{IDcolB}]
\]

The function computes the Hadamard product directly from \( A \) and \( B \) without forming \( R_1 AC'_1 \) or \( R_2 BC'_2 \) matrices.

**Value**

Returns a matrix containing the Hadamard product.

**Examples**

```r
require(tensorEVD)

# (a) Example 1. Indexing using row/column names
# Generate rectangular matrices A (nrowA x ncolA) and B (nrowB x ncolB)
nA = c(10,15)
nB = c(12,8)
B = matrix(rnorm(nB[1]*nB[2]), nrow=nB[1])
dimnames(A) = list(paste0("row",seq(nA[1])), paste0("col",seq(nA[2])))
dimnames(B) = list(paste0("row",seq(nB[1])), paste0("col",seq(nB[2])))

# Define IDs for a Hadamard of size n1 x n2
n = c(1000,500)
IDrowA = sample(rownames(A), n[1], replace=TRUE)
IDrowB = sample(rownames(B), n[1], replace=TRUE)
IDcolA = sample(colnames(A), n[2], replace=TRUE)
IDcolB = sample(colnames(B), n[2], replace=TRUE)
K1 = Hadamard(A, B, IDrowA, IDrowB, IDcolA, IDcolB, make.dimnames=TRUE)

# (it must equal to:)
dimnames(K2) = list(paste0("IDrowA",":\",IDrowB), paste0("IDcolA",":\",IDcolB))
all.equal(K1,K2)

# (b) Example 2. Indexing using integers
# Generate squared symmetric matrices A and B
nA = 20
nB = 15
A = tcrossprod(matrix(rnorm(nA*nA), nrow=nA))
```

B = tcrossprod(matrix(rnorm(nB*nB), nrow=nB))

# Define IDs for a Hadamard of size n x n
n = 1000
IDA = sample(seq(nA), n, replace=TRUE)
IDB = sample(seq(nB), n, replace=TRUE)

K1 = Hadamard(A, B, IDA, IDB)

# (it must equal to:)
K2 = A[IDA,IDA]*B[IDB,IDB]
all.equal(K1,K2)

# (c) Inplace calculation
# overwrite the output at the same address as the input:
IDB = sample(seq(nB), nA, replace=TRUE)
K1 = A[]  # copy of A to be used as input
add = pryr::address(K1)  # address of K on entry
K1 = Hadamard(K1, B, IDrowB=IDB)
pryr::address(K1) == add  # on exit, K was moved to a different address

K2 = A[]
add = pryr::address(K2)
K2 = Hadamard(K2, B, IDrowB=IDB, inplace=TRUE)
pryr::address(K2) == add  # on exit, K remains at the same address
all.equal(K1,K2)

Kronecker product

Description

Computes the direct Kronecker product between two matrices

Usage

Kronecker(A, B, rows = NULL, cols = NULL,
          make.dimnames = FALSE, drop = TRUE,
          inplace = FALSE)

Arguments

A (numeric) Left numeric matrix
B (numeric) Right numeric matrix
rows (integer) Index which rows of the Kronecker are to be returned. They must range from 1 to nrow(A)*nrow(B). Default rows=NULL will return all the rows
Kronecker product

cols  
(int) Index which columns of the Kronecker are to be returned. They must range from 1 to ncol(A)*ncol(B). Default cols=NULL return all the columns.

drop  
Either TRUE or FALSE to whether return a uni-dimensional vector when output is a matrix with either 1 row or 1 column as per the rows and cols arguments.

make.dimnames  
TRUE or FALSE to whether add rownames and colnames attributes to the output.

inplace  
TRUE or FALSE to whether operate directly on one input matrix (A or B) when the other one is a scalar. This is possible only when rows=NULL and cols=NULL. When TRUE the output will be overwritten on the same address occupied by the input that is not scalar. Default inplace=FALSE.

Details

For any two matrices $A = \{a_{ij}\}$ of dimensions $m \times n$ and $B = \{b_{ij}\}$ of dimensions $p \times q$, the direct Kronecker product between them is a matrix defined as the block matrix

$$A \otimes B = \{a_{ij}B\}$$

which is of dimensions $mp \times nq$.

A sub-matrix formed by selecting specific rows and columns from the Kronecker can be obtained by pre- and post- multiplication with incidence matrices

$$R(A \otimes B)C'$$

where $R$ is an incidence matrix mapping from rows of the resulting sub-matrix to rows of the Kronecker product, and $C$ is an incidence matrix mapping from columns of the resulting sub-matrix to columns of the Kronecker product. This sub-matrix of the Kronecker can be obtained by matrix indexing as

$$\text{Kronecker}(A,B)[\text{rows, cols}]$$

where rows and cols are integer vectors whose entries are, respectively, the row and column number of the Kronecker that are mapped at each row of $R$ and $C$.

The function computes this sub-matrix of the Kronecker product directly from $A$ and $B$ without forming the whole Kronecker product. This is very useful if a relatively small number of row/columns are to be selected.

Value

Returns the Kronecker product matrix. It can be a sub-matrix of it as per the rows and cols arguments.

Examples

```r
require(tensorEVD)

# (a) Kronecker product of 2 vectors
A = rnorm(3)
B = rnorm(2)
```
Multivariate variance matrix

Multivariate variance matrix penalization

Description

Ridge penalization of a multi-variate (co)variance matrix taking the form of either a Kronecker or Hadamard product

Usage

Kronecker_cov(Sigma = 1, K, Theta, swap = FALSE,
             rows = NULL, cols = NULL,
             drop = TRUE, inplace = FALSE)
Hadamard_cov(Sigma = 1, K, Theta, IDS, IDK, 
    drop = TRUE, inplace = FALSE)

**Arguments**

- **Sigma** (numeric) A variance matrix among features. If is scalar, a scaled identity matrix with the same dimension as Theta is used.
- **K** (numeric) Variance matrix among subjects.
- **Theta** (numeric) A diagonal-shifting parameter, value to be added to the diagonals of the resulting (co)variance matrix. It should be a (symmetric) matrix with the same dimension as Sigma.
- **rows** (integer) Index which rows of the (Kronecker product) (co)variance matrix are to be returned. Default `rows=NULL` will return all the rows.
- **cols** (integer) Index which columns of the (Kronecker product) (co)variance are to be returned. Default `cols=NULL` return all the columns.
- **IDS** (integer/character) Vector with either indices or row names mapping from rows/columns of Sigma and Theta into the resulting (Hadamard product) (co)variance matrix.
- **IDK** (integer/character) Vector with either indices or row names mapping from rows/columns of K into the resulting (Hadamard product) (co)variance matrix.
- **swap** (logical) Either TRUE or FALSE (default) to whether swap the order of the matrices in the resulting (Kronecker product) (co)variance matrix.
- **drop** (logical) Either TRUE or FALSE to whether return a uni-dimensional vector when output is a matrix with either 1 row or 1 column as per the rows and cols arguments.
- **inplace** (logical) Either TRUE or FALSE to whether operate directly on matrix K when Sigma and Theta are scalars. This is possible only when `rows=NULL` and `cols=NULL`. When TRUE the output will be overwritten on the same address occupied by K. Default `inplace=False`.

**Details**

Assume that a multi-variate random matrix $X$ with $n$ subjects in rows and $p$ features in columns follows a matrix Gaussian distribution with certain matrix of means $M$ and variance matrix $K$ of dimension $n \times n$ between subjects, and $\Sigma$ of dimension $p \times p$ between features.

**Kronecker product form.**

The random variable $x = vec(X)$, formed by stacking columns of $X$, is a vector of length $np$ that also follow a Gaussian distribution with mean $vec(M)$ and (co)variance covariance matrix taking the Kronecker form

$$\Sigma \otimes K$$

In the uni-variate case, the problem of near-singularity can be alleviated by penalizing the variance matrix $K$ by adding positive elements $\theta$ to its diagonal, i.e., $K + \theta I$, where $I$ is an identity matrix.
The same can be applied to the multi-variate case where the Kronecker product (co)variance matrix is penalized with $\Theta = \{\theta_{ij}\}$ of dimensions $p \times p$, where diagonal entries will penalize within feature $i$ and off-diagonals will penalize between features $i$ and $j$. This is,

$$\Sigma \otimes K + \Theta \otimes I$$

The second Kronecker summand $\Theta \otimes I$ is a sparse matrix consisting of non-zero diagonal and sub-diagonals. The Kronecker_cov function derives the penalized Kronecker (co)variance matrix by computing densely only the first Kronecker summand $\Sigma \otimes K$, and then calculating and adding accordingly only the non-zero entries of $\Theta \otimes I$.

*Note:* Swapping the order of the matrices in the above Kronecker operations will yield a different result. In this case the penalized matrix

$$K \otimes \Sigma + I \otimes \Theta$$

corresponds to the penalized multi-variate (co)variance matrix of the transposed of the above multi-variate random matrix $X$, now with features in rows and subjects in columns. This can be achieved by setting swap=TRUE in the Kronecker_cov function.

**Hadamard product form.**

Assume the random variable $x_0$ is a subset of $x$ containing entries corresponding to specific combinations of subjects and features, then the (co)variance matrix of the vector $x_0$ will be a Hadamard product formed by the entry-wise product of only the elements of $\Sigma$ and $K$ involved in the combinations contained in $x_0$; this is

$$(Z_1 \Sigma Z'_1) \odot (Z_2 KZ'_2)$$

where $Z_1$ and $Z_2$ are incidence matrices mapping from entries of the random variable $x_0$ to rows (and columns) of $\Sigma$ and $K$, respectively. This (co)variance matrix can be obtained using matrix indexing (see help(Hadamard)), as

$$\text{Sigma}[\text{IDS}, \text{IDS}] * \text{K}[\text{IDK}, \text{IDK}]$$

where IDS and IDK are integer vectors whose entries are the row (and column) number of $\Sigma$ and $K$, respectively, that are mapped at each row of $Z_1$ and $Z_2$, respectively.

The penalized version of this Hadamard product (co)variance matrix will be

$$(Z_1 \Sigma Z'_1) \odot (Z_2 KZ'_2) + (Z_1 \Theta Z'_1) \odot (Z_2 IZ'_2)$$

The Hadamard_cov function derives this penalized (co)variance matrix using matrix indexing, as

$$\text{Sigma}[\text{IDS}, \text{IDS}] * \text{K}[\text{IDK}, \text{IDK}] + \text{Theta}[\text{IDS}, \text{IDS}] * \text{I}[\text{IDK}, \text{IDK}]$$

Likewise, this function computes densely only the first Hadamard summand and then calculates and adds accordingly only the non-zero entries of the second summand.
Multivariate variance matrix

Value

Returns the penalized (co)variance matrix formed either as a Kronecker or Hadamard product. For the Kronecker product case, it can be a sub-matrix of the Kronecker product as per the rows and cols arguments.

Examples

```r
require(tensorEVD)

# Generate rectangular some covariance matrices
n = 30;  p = 10
K = crossprod(matrix(rnorm(n*p), ncol=n))  # n x n matrix
Sigma = crossprod(matrix(rnorm(n*p), ncol=p))  # p x p matrix
Theta = crossprod(matrix(rnorm(n*p), ncol=p))  # p x p matrix

# Kronecker covariance
G1 = Kronecker_cov(Sigma, K, Theta = Theta)
# it must equal to:
D = diag(n)  # diagonal matrix of dimension n
G2 = Kronecker(Sigma, K) + Kronecker(Theta, D)
all.equal(G1,G2)

# (b) Swapping the order of the matrices
G1 = Kronecker_cov(Sigma, K, Theta, swap = TRUE)
# in this case the kronecker is swapped:
G2 = Kronecker(K, Sigma) + Kronecker(D, Theta)
all.equal(G1,G2)

# (c) Selecting specific entries of the output
# We want only some rows and columns
rows = c(1,3,5)
cols = c(10,30,50)
G1 = Kronecker_cov(Sigma, K, Theta, rows=rows, cols=cols)
# this can be preferable instead of:
G2 = (Kronecker(Sigma, K) + Kronecker(Theta, D))[rows,cols]
all.equal(G1,G2)

# (d) Inplace calculation
# overwrite the output at the same address as the input:
G1 = K[]  # copy of K to be used as input
add = pryr::address(G1)  # address of G on entry
G1 = Kronecker_cov(Sigma=0.5, G1, Theta=1.5)
pryr::address(G1) == add  # on exit, G was moved to a different address
G2 = K[]
add = pryr::address(G2)
```
G2 = Kronecker_cov(Sigma=0.5, G2, Theta=1.5, inplace=TRUE)
pryr::address(G2) == add  # on exit, G remains at the same address
all.equal(G1,G2)

# ==============================================  # Hadamard covariance
# Define IDs for a Hadamard of size m x m
# m = 1000
IDS = sample(1:p, m, replace=TRUE)
IDK = sample(1:n, m, replace=TRUE)

G1 = Hadamard_cov(Sigma, K, Theta, IDS=IDS, IDK=IDK)
G2 = Sigma[IDS,IDS]*K[IDK,IDK] + Theta[IDS,IDS]*D[IDK,IDK]
all.equal(G1,G2)

# (b) Inplace calculation
# overwrite the output at the same address as the input:
G1 = K[]  # copy of K to be used as input
add = pryr::address(G1)  # address of G on entry
G1 = Hadamard_cov(Sigma=0.5, G1, Theta=1.5, IDS=rep(1,n))
pryr::address(G1) == add  # on exit, G was moved to a different address

G2 = K[]
add = pryr::address(G2)
G2 = Hadamard_cov(Sigma=0.5, G2, Theta=1.5, IDS=rep(1,n), inplace=TRUE)
pryr::address(G2) == add  # on exit, G remains at the same address
all.equal(G1,G2)

---

Tensor EVD

---

**Description**

Fast eigen value decomposition (EVD) of the Hadamard product of two matrices

**Usage**

```r
tensorEVD(K1, K2, ID1, ID2, alpha = 1.0,
          EVD1 = NULL, EVD2 = NULL,
          d.min = .Machine$double.eps,
          make.dimnames = FALSE, verbose = FALSE)
```

**Arguments**

- **K1, K2**  (numeric) Covariance structure matrices
Tensor EVD

ID1 (character/integer) Vector of length $n$ with either names or indices mapping from rows/columns of $K_1$ into the resulting tensor product

ID2 (character/integer) Vector of length $n$ with either names or indices mapping from rows/columns of $K_2$ into the resulting tensor product

alpha (numeric) Proportion of variance of the tensor product to be explained by the tensor eigenvectors

EVD1 (list) (Optional) Eigenvectors and eigenvalues of $K_1$ as produced by the eigen function

EVD2 (list) (Optional) Eigenvectors and eigenvalues of $K_2$ as produced by the eigen function

d.min (numeric) Tensor eigenvalue threshold. Default is a numeric zero. Only eigenvectors with eigenvalue passing this threshold are returned

make.dimnames TRUE or FALSE to whether add rownames and colnames attributes to the output

verbose TRUE or FALSE to whether show progress

Details

Let the $n \times n$ matrix $K$ to be the Hadamard product (aka element-wise or entry-wise product) involving two smaller matrices $K_1$ and $K_2$ of dimensions $n_1$ and $n_2$, respectively,

$$K = (Z_1 K_1 Z_1') \odot (Z_2 K_2 Z_2')$$

where $Z_1$ and $Z_2$ are incidence matrices mapping from rows (and columns) of the resulting Hadamard to rows (and columns) of $K_1$ and $K_2$, respectively.

Let the eigenvalue decomposition (EVD) of $K_1$ and $K_2$ to be $K_1 = V_1 D_1 V_1'$ and $K_2 = V_2 D_2 V_2'$. Using properties of the Hadamard and Kronecker products, an EVD of the Hadamard product $K$ can be approximated using the EVD of $K_1$ and $K_2$ as

$$K = V D V'$$

where $D = D_1 \otimes D_2$ is a diagonal matrix containing $N = n_1 \times n_2$ tensor eigenvalues $d_1 \geq \ldots \geq d_N \geq 0$ and $V = (Z_1 \star Z_2)(V_1 \otimes V_2) = [v_1, \ldots, v_N]$ is matrix containing $N$ tensor eigenvectors $v_k$; here the term $Z_1 \star Z_2$ is the "face-splitting product" (aka "transposed Khatri–Rao product") of matrices $Z_1$ and $Z_2$.

Each tensor eigenvector $k$ is derived separately as a Hadamard product using the corresponding $i(k)$ and $j(k)$ eigenvectors $v_{1i(k)}$ and $v_{2j(k)}$ from $V_1$ and $V_2$, respectively, this is

$$v_k = (Z_1 v_{1i(k)}) \odot (Z_2 v_{2j(k)})$$

The tensorEVD function derives each of these eigenvectors $v_k$ by matrix indexing using integer vectors ID1 and ID2. The entries of these vectors are the row (and column) number of $K_1$ and $K_2$ that are mapped at each row of $Z_1$ and $Z_2$, respectively.
**Value**

Returns a list object that contains the elements:

- **values**: (vector) resulting tensor eigenvalues.
- **vectors**: (matrix) resulting tensor eigenvectors.
- **totalVar**: (numeric) total variance of the tensor matrix product.

**Examples**

```r
require(tensorEVD)
set.seed(195021)

# Generate matrices K1 and K2 of dimensions n1 and n2
n1 = 10; n2 = 15
K1 = crossprod(matrix(rnorm(n1*(n1+10)), ncol=n1))
K2 = crossprod(matrix(rnorm(n2*(n2+10)), ncol=n2))

# (a) Example 1. Full design (Kronecker product)
ID1 = rep(seq(n1), each=n2)
ID2 = rep(seq(n2), times=n1)

# Direct EVD of the Hadamard product
K = K1[ID1,ID1]*K2[ID2,ID2]
EVD0 = eigen(K)

# Tensor EVD using K1 and K2
EVD = tensorEVD(K1, K2, ID1, ID2)

# Eigenvectors and eigenvalues are numerically equal
all.equal(EVD0$values, EVD$values)
all.equal(abs(EVD0$vectors), abs(EVD$vectors))

# (b) If a proportion of variance explained is specified,
# only the eigenvectors needed to explain such proportion are derived
alpha = 0.95
EVD = tensorEVD(K1, K2, ID1, ID2, alpha=alpha)
dim(EVD$vectors)

# For the direct EVD
varexp = cumsum(EVD0$values/sum(EVD0$values))
index = 1:which.min(abs(varexp-alpha))
dim(EVD0$vectors[,index])

# (c) Example 2. Incomplete design (Hadamard product)
# Eigenvectors and eigenvalues are no longer equivalent
n = n1*n2  # Sample size n
ID1 = sample(seq(n1), n, replace=TRUE)  # Randomly sample of ID1
ID2 = sample(seq(n2), n, replace=TRUE)  # Randomly sample of ID2

K = K1[ID1,ID1]*K2[ID2,ID2]
EVD0 = eigen(K)
EVD = tensorEVD(K1, K2, ID1, ID2)
```
all.equal(EVD0$values, EVD$values)
all.equal(abs(EVD0$vectors), abs(EVD$vectors))

# However, the sum of the eigenvalues is equal to the trace(K)
c(sum(EVD0$values), sum(EVD$values), sum(diag(K))))

# And provide the same approximation for K
K01 = EVD0$vectors%*%diag(EVD0$values)%*%t(EVD0$vectors)
K02 = EVD$vectors%*%diag(EVD$values)%*%t(EVD$vectors)
c(all.equal(K,K01), all.equal(K,K02))

# When n is different from N=n1*n2, both methods provide different
# number or eigenvectors/eigenvalues. The eigen function provides
# a number of eigenvectors equal to the minimum between n and N
# for the tensorEVD, this number is always N

# (d) Sample size n being half of n1 x n2
n = n1*n2/2
ID1 = sample(seq(n1), n, replace=TRUE)
ID2 = sample(seq(n2), n, replace=TRUE)
K = K1[ID1,ID1]*K2[ID2,ID2]
EVD0 = eigen(K)
EVD = tensorEVD(K1, K2, ID1, ID2)
c(eigen=sum(EVD0$values>1E-10), tensorEVD=sum(EVD$values>1E-10))

# (e) Sample size n being twice n1 x n2
n = n1*n2*2
ID1 = sample(seq(n1), n, replace=TRUE)
ID2 = sample(seq(n2), n, replace=TRUE)
K = K1[ID1,ID1]*K2[ID2,ID2]
EVD0 = eigen(K)
EVD = tensorEVD(K1, K2, ID1, ID2)
c(eigen=sum(EVD0$values>1E-10), tensorEVD=sum(EVD$values>1E-10))
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