Package ‘rstiefel’

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Type Package

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Description

Package: rstiefel
Type: Package
Version: 1.0.0
Date: 2019-02-18
License: GPL-3

Author(s)

Peter Hoff
Alex Franks
**Description**

A curvilinear search on the Stiefel manifold (Wen and Yin 2013, Algo 1)

**Usage**

```r
lineSearch(f, df, X, rho1, rho2, tauStart, maxIters = 20)
```

**Arguments**

- `f`: A function \( V(n, p) \rightarrow \mathbb{R}^1 \)
- `df`: A function \( V(n, p) \rightarrow \mathbb{R}^1 \)
- `X`: An \( n \times p \) semi-orthogonal matrix (starting point)
- `rho1`: Parameter for Armijo condition. Between 0 and 1 and usually small, e.g., < 0.1
- `rho2`: Parameter for Wolfe condition. Between 0 and 1 usually large, > 0.9
- `tauStart`: Initial step size
- `maxIters`: Maximum number of iterations

**Value**

A list containing: `Y`, the semi-orthogonal matrix satisfying the Armijo-Wolfe conditions and `tau`: the stepsize satisfying these conditions

**Author(s)**

Alexander Franks
References

(Wen and Yin, 2013)

Examples

```r
N <- 10  
P <- 2  
M <- diag(10:1)  
F <- function(V) { - sum(diag(t(V) %*% M %*% V)) }  
dF <- function(V) { - 2*M %*% V }  
X <- rustiefel(N, P)  
res <- lineSearch(F, dF, X, rho1=0.1, rho2=0.9, tauStart=1)
```

Description

A curvilinear search on the Stiefel manifold with BB steps (Wen and Yin 2013, Algo 2) This is based on the line search algorithm described in (Zhang and Hager, 2004)

Usage

```r
lineSearchBB(F, X, xprev, G_x, G_xprev, rho, C, maxIters = 20)
```

Arguments

- **F**: A function \( V(n, p) \rightarrow \mathbb{R} \)
- **X**: An \( n \times p \) semi-orthogonal matrix (the current)
- **xprev**: An \( n \times p \) semi-orthogonal matrix (the previous)
- **G_x**: An \( n \times p \) matrix with \( (G_x)_{ij} = \frac{dF(X)}{dX_{ij}} \)
- **G_xprev**: An \( n \times p \) matrix with \( (G_{xprev})_{ij} = \frac{dF(X_{prev})}{dX_{prev}_{ij}} \)
- **rho**: Convergence parameter, usually small (e.g. 0.1)
- **C**: \( C_{t+1} = (\eta t + F(X_{t+1}))/Q_{t+1} \) See section 3.2 in Wen and Yin, 2013
- **maxIters**: Maximum number of iterations

Value

A list containing \( Y \): a semi-orthogonal matrix \( Y_{\text{tau}} \) which satisfies convergence criteria (Eqn 29 in Wen & Yin ‘13), and \( \tau \): the stepsize satisfying these criteria
**NullC**

*Author(s)*

Alexander Franks

*References*

(Wen and Yin, 2013) and (Zhang and Hager, 2004)

*Examples*

```r
N <- 10
P <- 2
M <- diag(1:1)
F <- function(V) { - sum(diag(t(V) %*% M %*% V)) }
dF <- function(V) { - 2*M %*% V }
Xprev <- rustiefel(N, P)
G_xprev <- dF(Xprev)
X <- rustiefel(N, P)
G_x <- dF(X)
Xprev <- dF(X)
res <- lineSearchBB(F, X, Xprev, G_x, G_xprev, rho=0.1, C=F(X))
```

---

**Description**

Given a matrix \( M \), find a matrix \( N \) giving a basis for the null space. This is a modified version of Null from the package MASS.

**Usage**

`NullC(M)`

**Arguments**

- **M**: input matrix.

**Value**

an orthonormal matrix such that \( t(N) %*% M \) is a matrix of zeros.

**Note**

The MASS function `Null(matrix(0,4,2))` returns a 4\( \times \)2 matrix, whereas `NullC(matrix(0,4,2))` returns `diag(4)`. 
Author(s)

Peter Hoff

Examples

```
# NullC(matrix(0,4,2))

## The function is currently defined as
## function (M)
## {
##  tmp <- qr(M)
##  set <- if (tmp$rank == 0L)
##    1L:nrow(M)
##  else -(1L:tmp$rank)
##  qr.Q(tmp, complete = TRUE)[, set, drop = FALSE]
## }
```

Description

Find a local optimum of a function defined on the stiefel manifold using algorithms described in Wen and Yin (2013).

Usage

```
opstiefel(F, df, vinit, method = "bb", searchparams = NULL, tol = 1e-12,
          maxiters = 100, verbose = FALSE, maxlineSearchIters = 20)
```

Arguments

- **F**
  A function V(P, S) \rightarrow \mathbb{R}^1

- **df**
  A function to compute the gradient of F. Returns a P \times S matrix with \frac{dF(X)_{ij}}{dX_{ij}}

- **vinit**
  The starting point on the stiefel manifold for the optimization

- **method**
  Line search type: "bb" or curvilinear

- **searchparams**
  List of parameters for the line search algorithm. If the line search algorithm is the standard curvilinear search than the search parameters are rho1 and rho2. If the line search algorithm is "bb" then the parameters are rho and eta.

- **tol**
  Convergence tolerance. Optimization stops when Fprime < abs(tol), an approximate stationary point.

- **maxIters**
  Maximum iterations for each gradient step

- **verbose**
  Boolean indicating whether to print function value and iteration number at each step.
maxLineSearchIters
    Maximum iterations for for each line search (one step in the gradient descent algorithm)

Value
    A stationary point of \( F \) on the Stiefel manifold.

Author(s)
    Alexander Franks

References
    (Wen and Yin, 2013)

Examples
    ## Find the first eigenspace spanned by the first \( P \) eigenvectors for a
    ## matrix \( M \). The size of the matrix has been kept small and the tolerance
    ## has been raised to keep the runtime
    ## of this example below the CRAN submission threshold.

    N <- 500
    P <- 3
    Lam <- diag(c(10, 5, 3, rep(1, N-P)))
    U <- rustiefel(N, N)
    M <- U %*% Lam %*% t(U)
    
    F <- function(V) { - sum(diag(t(V) %*% M %*% V)) }
    dF <- function(V) { - 2*M %*% V }
    V = optStiefel(F, dF, Vinit=rustiefel(N, P),
                   method="curvilinear",
                   searchParams=list(rho1=0.1, rho2=0.9, tau=1), tol=1e-4)
    
    print(sprintf("Sum of first %d eigenvalues is %.f", P, -F(V)))

---

**rbing.matrix.gibbs**

*Gibbs Sampling for the Matrix-variate Bingham Distribution*

**Description**

Simulate a random orthonormal matrix from the Bingham distribution using Gibbs sampling.

**Usage**

*rbing.matrix.gibbs(A, B, X)*
Arguments

A  a symmetric matrix.
B  a diagonal matrix with decreasing entries.
X  the current value of the random orthonormal matrix.

Value

a new value of the matrix X obtained by Gibbs sampling.

Note

This provides one Gibbs scan. The function should be used iteratively.

Author(s)

Peter Hoff

References

Hoff(2009)

Examples

```
Z<-matrix(rnorm(10*5),10,5) ; A<-t(Z)%*%Z
B<-diag(sort(rexp(5),decreasing=TRUE))
U<-rbing.Op(A,B)
U<-rbing.matrix.gibbs(A,B,U)

## The function is currently defined as
function (A, B, X)
{
  m <- dim(X)[1]
  R <- dim(X)[2]
  if (m > R) {
    for (r in sample(seq(1, R, length = R))) {
      N <- NullC(X[, -r])
      An <- B[r, r] * t(N) %*% A %*% N
      X[, r] <- N %*% rbing.vector.gibbs(An, t(N) %*% X[, r])
    }
  }
  if (m == R) {
    for (s in seq(1, R, length = R)) {
      r <- sort(sample(seq(1, R, length = R), 2))
      N <- NullC(X[, -r])
      An <- t(N) %*% A %*% N
      X[, r] <- N %*% rbing.Op(An, B[r, r])
    }
  }
  X
```
Simulate a 2*2 Orthogonal Random Matrix

Description

Simulate a 2*2 random orthogonal matrix from the Bingham distribution using a rejection sampler.

Usage

\texttt{rbing.02}(A, B, a = \texttt{NULL}, E = \texttt{NULL})

Arguments

\begin{itemize}
  \item [A] a symmetric matrix.
  \item [B] a diagonal matrix with decreasing entries.
  \item [a] sum of the eigenvalues of A, multiplied by the difference in B-values.
  \item [E] eigenvectors of A.
\end{itemize}

Value

A random 2x2 orthogonal matrix simulated from the Bingham distribution.

Author(s)

Peter Hoff

References

Hoff(2009)

Examples

```r
## The function is currently defined as
function (A, B, a = \texttt{NULL}, E = \texttt{NULL})
{
  if (is.null(a)) {
    a <- la * (B[1, 1] - B[2, 2])
    E <- diag(2)
    if (A[1, 2] != 0) {
      E <- cbind(c(0.5 * (trA + la) - A[2, 2], A[1, 2]),
                 c(0.5 * (trA - la) - A[2, 2], A[1, 2]))
      E[, 1] <- E[, 1]/sqrt(sum(E[, 1]^2))
    }
    return(E)
  }
  return(null)
}
```
E[, 2] <- E[, 2]/sqrt(sum(E[, 2]^2))

b <- min(1/a^2, 0.5)
beta <- 0.5 - b
lrmx <- a
if (beta > 0) {
lrmx <- lrmx + beta * (log(beta/a) - 1)
}
lr <- -Inf
while (lr < log(runif(1))) {
w <- rbeta(1, 0.5, b)
lr <- a * w + beta * log(1 - w) - lrmx
}
u <- c(sqrt(w), sqrt(1 - w)) * (-1)^rbinom(2, 1, 0.5)
x1 <- E %*% u
x2 <- (x1[2:1] * c(-1, 1) * (-1)^rbinom(1, 1, 0.5))
cbind(x1, x2)

rbing.Op

*Simulate a p*p Orthogonal Random Matrix*

**Description**

Simulate a p*p random orthogonal matrix from the Bingham distribution using a rejection sampler.

**Usage**

rbing.Op(A, B)

**Arguments**

A

a symmetric matrix.

B

a diagonal matrix with decreasing entries.

**Value**

A random pxp orthogonal matrix simulated from the Bingham distribution.

**Note**

This only works for small matrices, otherwise the sampler will reject too frequently to be useful.

**Author(s)**

Peter Hoff
References

Hoff(2009)

Examples

```
Z<-matrix(rnorm(10*5),10,5) ; A<-t(Z)%%Z
B<-diag(sort(rexp(5),decreasing=TRUE))
U<-rbing.Op(A,B)
U<-rbing.matrix.gibbs(A,B,U)
```

```
## The function is currently defined as
function (A, B)
{
    b <- diag(B)
    bmx <- max(b)
    bmn <- min(b)
    if(bmx>bmn)
        {
            A <- A * (bmx - bmn)
            b <- (b - bmn)/(bmx - bmn)
            vlA <- eigen(A)$val
            diag(A) <- diag(A) - vlA[1]
            vlA <- eigen(A)$val
            nu <- max(dim(A)[1] + 1, round(-vlA[length(vlA)]))
            del <- nu/2
            M <- solve(diag(del, nrow = dim(A)[1]) - A/2)
            rej <- TRUE
            cholM <- chol(M)
            nrej <- 0
            while (rej) {
                Z <- matrix(rnorm(nu * dim(M)[1]), nrow = nu, ncol = dim(M)[1])
                Y <- Z %*% cholM
                tmp <- eigen(t(Y) %*% Y)
                U <- tmp$vec %*% diag((-1)*rbinom(dim(A)[1], 1, 0.5))
                L <- diag(tmp$val)
                D <- diag(b) - L
                lrr <- sum(diag((D %*% t(U) %*% A %*% U))) - sum(sort(diag(-D)) * vlA)
                rej <- (log(runif(1)) > lrr)
                nrej <- nrej + 1
            }
        }
    if(bmx==bmn) { U<-rustiefel(dim(A)[1],dim(A)[1]) }
    U
}
```
rbing.vector.gibbs  Gibbs Sampling for the Vector-variate Bingham Distribution

Description

Simulate a random normal vector from the Bingham distribution using Gibbs sampling.

Usage

rbing.vector.gibbs(A, x)

Arguments

A  a symmetric matrix.

x  the current value of the random normal vector.

Value

a new value of the vector x obtained by Gibbs sampling.

Note

This provides one Gibbs scan. The function should be used iteratively.

Author(s)

Peter Hoff

References

Hoff(2009)

Examples

## The function is currently defined as
rbing.vector.gibbs <-
function(A, x)
{
  # simulate from the vector bmf distribution as described in Hoff(2009)
  # this is one gibbs step, and must be used iteratively
  evdA<-eigen(A,symmetric=TRUE)
  E<-evdA$vec
  l<-evdA$val

  y<-t(E)%*%x
  xc<-E%*%ry_bing(y,1)
  x/sqrt(sum(x^2))
  # one improvement might be a rejection sampler

Description
Simulate a random orthonormal matrix from the Bingham distribution using Gibbs sampling.

Usage
rbmf.matrix.gibbs(A, B, C, X)

Arguments
- **A**: a symmetric matrix.
- **B**: a diagonal matrix with decreasing entries.
- **C**: a matrix with the same dimension as X.
- **X**: the current value of the random orthonormal matrix.

Value
a new value of the matrix X obtained by Gibbs sampling.

Note
This provides one Gibbs scan. The function should be used iteratively.

Author(s)
Peter Hoff

References
Hoff(2009)
Examples

```r
## The function is currently defined as
function HaL bL cL xI {
  m <- dim(X)[1]
  R <- dim(X)[2]
  if (m > R) {
    for (r in sample(seq(1, R, length = R))) {
      N <- NullC(X[, -r])
      An <- B[r, r] * t(N) %*% (A) %*% N
      cn <- t(N) %*% C[, r]
      X[, r] <- N %*% rbmf.vector.gibbs(An, cn, t(N) %*%
        X[, r])
    }
  }
  if (m == R) {
    for (s in seq(1, R, length = R)) {
      r <- sort(sample(seq(1, R, length = R), 2))
      N <- NullC(X[, -r])
      An <- t(N) %*% A %*% N
      Cn <- t(N) %*% C[, r]
      X[, r] <- N %*% rbmf.02(An, B[r, r], Cn)
    }
  }
  X
}
```

---

**Simulate a 2*2 Orthogonal Random Matrix**

**Description**

Simulate a 2*2 random orthogonal matrix from the Bingham-von Mises-Fisher distribution using a rejection sampler.

**Usage**

```
rbmf.02(A, B, C, env = FALSE)
```

**Arguments**

- **A**: a symmetric matrix.
- **B**: a diagonal matrix with decreasing entries.
- **C**: a 2x2 matrix.
- **env**: which rejection envelope to use, Bingham (bingham) or von Mises-Fisher (mf)?
Value

A random 2x2 orthogonal matrix simulated from the Bingham-von Mises-Fisher distribution.

Author(s)

Peter Hoff

References

Hoff(2009)

Examples

```r
## The function is currently defined as
function (A, B, C, env = FALSE)
{
  sC <- svd(C)
d1 <- sum(sC$d)
eA <- eigen(A)
ab <- sum(eA$val * diag(B))
  if (d1 <= ab | env == "bingham") {
    lrmx <- sum(sC$d)
    lr <- -Inf
    while (lr < log(runif())) {
      X <- rbing.02(A, B, a = (eA$val[1] - eA$val[2]) *
        (B[1, 1] - B[2, 2]), E = eA$vec)
      lr <- sum(diag(t(X) %*% C)) - lrmx
    }
  }
  if (d1 > ab | env == "mf") {
    lrmx <- sum(eA$val * sort(diag(B), decreasing = TRUE))
    lr <- -Inf
    while (lr < log(runif())) {
      X <- rmf.matrix(C)
      lr <- sum(diag(B %*% t(X) %*% A %*% X)) - lrmx
    }
  }
  X
}
```

Description

Simulate a random normal vector from the Bingham-von Mises-Fisher distribution using Gibbs sampling.
Usage

rbmf.vector.gibbs(A, c, x)

Arguments

A  a symmetric matrix.
c  a vector with the same length as x.
x  the current value of the random normal vector.

Value

a new value of the vector x obtained by Gibbs sampling.

Note

This provides one Gibbs scan. The function should be used iteratively.

Author(s)

Peter Hoff

References

Hoff(2009)

Examples

```r
## The function is currently defined as
function (A, c, x)
{
  evdA <- eigen(A)
  E <- evdA$vec
  l <- evdA$val
  y <- t(E) %% x
  d <- t(E) %% c
  x <- E %% ry_bmf(y, l, d)
  x/sqrt(sum(x^2))
}
```
Description

Simulate a random orthonormal matrix from the von Mises-Fisher distribution.

Usage

```r
rmf.matrix(M)
```

Arguments

- `M` a matrix.

Value

an orthonormal matrix of the same dimension as `M`.

Author(s)

Peter Hoff

References

Hoff (2009)

Examples

```r
## The function is currently defined as
Z <- matrix(rnorm(10*5),10,5)

U <- rmf.matrix(Z)
U <- rmf.matrix.gibbs(Z,U)
```

```r
function (M)
{
  if (dim(M)[2] == 1) {
    X <- rmf.vector(M)
  }
  if (dim(M)[2] > 1) {
    svdM <- svd(M)
    H <- svdM$u %*% diag(svdM$d)
    m <- dim(H)[1]
    R <- dim(H)[2]
    cmet <- FALSE
    rej <- 0
    while (!cmet) {
```
U <- matrix(0, m, R)
U[, 1] <- rmf.vector(H[, 1])
lr <- 0
for (j in seq(2, R, length = R - 1)) {
  N <- NULLC(U[, seq(1, j - 1, length = j - 1)])
  x <- rmf.vector(t(N) %*% H[, j])
  U[, j] <- N %*% x
  if (svdM$d[j] > 0) {
    xn <- sqrt(sum((t(N) %*% H[, j])^2))
    xd <- sqrt(sum(H[, j]^2))
    lbr <- log(besselI(xn, 0.5 * (m - j - 1), expon.scaled = TRUE)) -
          log(besselI(xd, 0.5 * (m - j - 1), expon.scaled = TRUE))
    if (is.na(lbr)) {
      lbr <- 0.5 * (log(xd) - log(xn))
    }
    lr <- lr + lbr + (xn - xd) + 0.5 * (m - j - 1) * (log(xd) - log(xn))
  }
}
cmet <- (log(runif(1)) < lr)
rej <- rej + (1 - 1 * cmet)
X <- U %*% t(svd(M)$v)
X

rmf.matrix.gibbs

Gibbs Sampling for the Matrix-variate von Mises-Fisher Distribution

Description
Simulate a random orthonormal matrix from the matrix von Mises-Fisher distribution using Gibbs
sampling.

Usage
rmf.matrix.gibbs(M, X, rscol = NULL)

Arguments

M
  a matrix.
X
  the current value of the random orthonormal matrix.

rscol
  the number of columns to update simultaneously.

Value

a new value of the matrix X obtained by Gibbs sampling.
**rmf.vector**  
*

**Note**

This provides one Gibbs scan. The function should be used iteratively.

**Author(s)**

Peter Hoff

**References**

Hoff(2009)

**Examples**

```r
Z<-matrix(rnorm(10*5),10,5)
U<-rmf.matrix(Z)
U<-rmf.matrix.gibbs(Z,U)
```

```r
## The function is currently defined as
function (M, X, rscol = NULL)
{
  if (is.null(rscol)) {
    rscol <- max(2, min(round(log(dim(M)[1])), dim(M)[2]))
  }
  sM <- svd(M)
  H <- sM$su %*% diag(sM$sd)
  Y <- X %*% sM$u
  m <- dim(H)[1]
  R <- dim(H)[2]
  for (iter in 1:round(R/rscol)) {
    r <- sample(seq(1, R, length = R), rscol)
    N <- NULL(Y[, -r])
    y <- rmf.matrix(t(N) %*% H[, r])
    Y[, r] <- N %*% y
  }
  Y %*% t(sM$v)
}
```

**Description**

Simulate a random normal vector from the von Mises-Fisher distribution as described in Wood(1994).
Usage

```
rmf.vector(kmu)
```

Arguments

```
kmu a vector.
```

Value

```
a vector.
```

Author(s)

Peter Hoff

References

Wood(1994), Hoff(2009)

Examples

```R
## The function is currently defined as
function HkmuI {
  kap <- sqrt(sum(kmu^2))
  mu <- kmu/kap
  m <- length(mu)
  if (kap == 0) {
    u <- rnorm(length(kmu))
    u <- matrix(u/sqrt(sum(u^2)),m,1)
  }
  if (kap > 0) {
    if (m == 1) {
      u <- (-1)^rbinom(1, 1, 1/(1 + exp(2 * kap * mu)))
    }
    if (m > 1) {
      W <- rw(kap, m)
      V <- rnorm(m - 1)
      V <- V/sqrt(sum(V^2))
      x <- c((1 - W^2)^0.5 * t(V), W)
      u <- cbind(NullC(mu), mu) %% x
    }
  }
  u

}
```
Simulate a Uniformly Distributed Random Orthonormal Matrix

Description

Simulate a random orthonormal matrix from the uniform distribution on the Stiefel manifold.

Usage

```r
rustiefel(m, R)
```

Arguments

- `m` the length of each column vector.
- `R` the number of column vectors.

Value

an `m*R` orthonormal matrix.

Author(s)

Peter Hoff

References

Hoff (2007)

Examples

```r
# The function is currently defined as
function (m, R)
{
  X <- matrix(rnorm(m * R), m, R)
  tmp <- eigen(t(X) %*% X)
  X %*% (tmp$vec %*% sqrt(diag(1/tmp$val, nrow = R)) %*% t(tmp$vec))
}
```
**Description**

Auxilliary variable simulation for rejection sampling of \texttt{rmf.vector}, as described in Wood(1994).

**Usage**

\texttt{rw(kap, m)}

**Arguments**

- \texttt{kap} a positive scalar.
- \texttt{m} a positive integer.

**Value**

A number between zero and one.

**Author(s)**

Peter Hoff

**Examples**

\texttt{rw(pi,4)}

```r
## The function is currently defined as
function (kap, m)
{
  .C("rw", kap = as.double(kap), m = as.integer(m), w = double(1))$w
}
```

---

**Description**

C interface to perform a Gibbs update of \( y \) with invariant distribution proportional to \( \exp\left( \sum l y^2 \right) \) with respect to the uniform measure on the sphere.

**Usage**

\texttt{ry_bing(y, l)}
Arguments

<table>
<thead>
<tr>
<th>y</th>
<th>a normal vector.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>a vector.</td>
</tr>
</tbody>
</table>

Value

a normal vector.

Author(s)

Peter Hoff

References

Hoff (2009)

Examples

```
## The function is currently defined as
function (y, l)
{
  .C("ry_bing", y = as.double(y), l = as.double(l), n = as.integer(length(y)))$y
}
```

Description

C interface to perform a Gibbs update of \( y \) with invariant distribution proportional to \( \exp\left(\sum l \cdot y + 2 y \cdot d\right) \) with respect to the uniform measure on the sphere.

Usage

`ry_bmf(y, l, d)`

Arguments

<table>
<thead>
<tr>
<th>y</th>
<th>a normal vector.</th>
</tr>
</thead>
<tbody>
<tr>
<td>l</td>
<td>a vector.</td>
</tr>
<tr>
<td>d</td>
<td>a vector.</td>
</tr>
</tbody>
</table>

Value

a normal vector.
Author(s)

Peter Hoff

References

Hoff(2009)

Examples

```r
## The function is currently defined as
function (y, l, d)
{
  .C("ry_bmf", y = as.double(y), l = as.double(l), d = as.double(d),
      n = as.integer(length(y)))$y
}
```

---

tr  

*Compute the trace of a matrix*

---

**Description**

compute the trace of a square matrix

**Usage**

`tr(X)`

**Arguments**

- `X`  
  Square matrix
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