Package ‘hitandrun’

October 13, 2022

Type Package
Title ``Hit and Run'' and ``Shake and Bake'' for Sampling Uniformly from Convex Shapes
Version 0.5-6
Date 2022-05-26

URL https://github.com/gertvv/hitandrun
License GPL-3
LazyLoad yes
Imports rcdd (>= 1.1), stats
Suggests testthat (>= 0.8)
NeedsCompilation yes
Author Gert van Valkenhoef [aut, cre, cph],
Tommi Tervonen [aut]
Maintainer Gert van Valkenhoef <gert@gertvv.nl>
Repository CRAN
Date/Publication 2022-05-27 13:10:02 UTC

R topics documented:

hitandrun-package ......................................................... 2
bbReject ................................................................. 4
createBoundBox .......................................................... 5
createSeedPoint ......................................................... 6
createTransform ......................................................... 7
eliminateRedundant ..................................................... 8
hitandrun-package

"Hit and Run" sampling

Description

This package provides a "Hit and Run" sampler that generates a Markov chain whose stable state converges on the uniform distribution over a convex polytope. The polytope is given by a set of inequality constraints in standard linear programming form ($Ax \leq b$) and optionally a set of equality constraints. In addition, there is a "Shake and Bake" sampler to generate points from the boundary of such a shape.

Utilities are provided for sampling from subsets of the unit simplex (i.e. random variates that can be interpreted as weights satisfying certain constraints) and for specifying common constraints.

Details

hitandrun and shakeandbake now provide the most general interface for sampling from spaces defined by arbitrary linear equality and inequality constraints. The functions described in the following provide lower level functionality on which it is built.

har is the core "Hit and Run" sampler, sab is the core "Shake and Bake" sampler, bbReject is the bounding box rejection sampler, and simplex.sample samples uniformly from the unit simplex.

See simplex.createTransform and simplex.createConstraints for sampling from subsets of the unit simplex. Utilities to specify common constraints are described in harConstraints.

When the sampling space is restricted by different linear equality constraints, use solution.basis, createTransform, and transformConstraints. This is a generalization of the methods for sampling from the simplex.
Note

"Hit and Run" is a Markov Chain Monte Carlo (MCMC) method, so generated samples form a correlated time series. To get a uniform sample, you need $O^*(n^3)$ samples, where $n$ is the dimension of the sampling space.

Author(s)

Maintainer: Gert van Valkenhoef <gert@gertvv.nl>

References


See Also

hitandrun har
bbReject simplex.sample hypersphere.sample
solution.basis createTransform transformConstraints
simplex.createTransform simplex.createConstraints
harConstraints
createSeedPoint createBoundBox

Examples

```r
# Example: sample weight vectors where w_1 >= w_2 and w_1 >= w_3
n <- 3 # length of weight vector
constr <- mergeConstraints(
  ordinalConstraint(n, 1, 2),
  ordinalConstraint(n, 1, 3))
transform <- simplex.createTransform(n)
constr <- simplex.createConstraints(transform, constr)
seedPoint <- createSeedPoint(constr, homogeneous=TRUE)
N <- 1000
w <- har(seedPoint, constr, N=N * (n-1)^3, thin=(n-1)^3,
  homogeneous=TRUE, transform=transform)$samples
stopifnot(all(w[,1] >= w[,2]) && all(w[,1] >= w[,3]))
```
bbReject (Bounding box rejection sampler)

**Description**
Generates uniform random variates over a convex polytope defined by a set of linear constraints by generating uniform variates over a bounding box and rejecting those outside the polytope.

**Usage**
```
bbReject(lb, ub, constr, N, homogeneous=FALSE, transform=NULL)
```

**Arguments**
- `lb`: Lower bound for each dimension (not including homogeneous coordinate)
- `ub`: Upper bound for each dimension (not including homogeneous coordinate)
- `constr`: Constraint definition (see details)
- `N`: Number of samples to generate
- `homogeneous`: Whether constr and transform are given in homogeneous coordinate representation (see details)
- `transform`: Transformation matrix to apply to the generated samples (optional)

**Details**
See `har` for a description of the constraint definition and the homogeneous coordinate representation.

**Value**
A list, containing:
- `samples`: A matrix containing the generated samples as rows.
- `rejectionRate`: The mean number of samples rejected for each accepted sample.

**Author(s)**
Gert van Valkenhoef

**See Also**
- `createBoundBox`
- `harConstraints`
createBoundBox

Examples

# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("="", ","", ","")
constr <- list(constr=A, rhs=b, dir=d)

# create a bounding box that contains the polytope
lb <- c(0, 0)
ub <- c(1, 1)

# sample 10,000 points
samples <- bbReject(lb, ub, constr, 1E4)$samples

# Check dimension of result
stopifnot(dim(samples) == c(1E4, 2))

# Check that x_i >= 0
stopifnot(samples >= 0)

# Check that x_1 + x_2 <= 1
stopifnot(samples[,1] + samples[,2] <= 1)

plot(samples)

createBoundBox  Calculate a bounding box

Description

Calculate a bounding box around a polytope given by a set of linear constraints.

Usage

createBoundBox(constr, homogeneous=FALSE)

Arguments

constr  Constraint definition
homogeneous  Whether constr is given in homogeneous coordinate representation

Details

See har for a description of the constraint definition and the homogeneous coordinate representation.

This function uses findExtremePoints to find extreme points along each dimension.
createSeedPoint

Generate a seed point inside a polytope given by a set of linear constraints.

Usage

createSeedPoint(constr, homogeneous=FALSE, randomize=FALSE, method="slacklp")

Arguments

constr       Constraint definition
homogeneous  Whether constr is given in homogeneous coordinate representation
randomize    If TRUE, randomize the starting point
method       How to obtain the starting point: "slacklp" for a linear program that maximizes
             the minimum slack, or "vertices" for a weighted average of the vertices of the
             polytope

Description

Generate a seed point inside a polytope given by a set of linear constraints.

Examples

# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("<=", "<=", "<=")
constr <- list(constr=A, rhs=b, dir=d)

bb <- createBoundBox(constr)
stopifnot(bb$lb == c(0.0, 0.0))
stopifnot(bb$ub == c(1.0, 1.0))
createTransform

Details

See `har` for a description of the constraint definition and the homogeneous coordinate representation.

- The "slacklp" method solves a linear program that maximizes the minimum slack on the inequality constraints. When randomized, the slack on each constraint is randomly rescaled before maximization.
- The "vertices" method enumerates all vertices of the polytope and then calculates the weighted arithmetic mean of this set of points. If ‘randomize’ is set, the weights are randomly generated, otherwise they are all equal and the generated point is the centroid of the polytope.

Value

A coordinate vector in the appropriate coordinate system.

Author(s)

Gert van Valkenhoef

See Also

`har`
`findExtremePoints`
`findVertices`

Examples

```r
# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("="", ","", ",""")
constr <- list(constr=A, rhs=b, dir=d)

x0 <- createSeedPoint(constr)
stopifnot(x0 >= 0)
stopifnot(sum(x0) <= 1)
```

createTransform  

Create transformation matrices

Description

This function takes a basis, consisting of an \( n \times m \) change of basis matrix and an \( n \)-vector representing the origin of the \( m \)-space, and generates a matrix to transform points in the \( m \)-space, given in homogeneous coordinates, to the \( n \)-space.

The inverse transform can also be generated, and conversion can be to homogeneous coordinates instead of Cartesian ones.
Usage

createTransform(basis, inverse=FALSE, keepHomogeneous=inverse)

Arguments

- **basis**: Basis (and origin) for the \(m\)-space (see `solution.basis`)
- **inverse**: TRUE to convert from \(n\)-space coordinates to \(m\)-space coordinates
- **keepHomogeneous**: TRUE to convert to homogeneous coordinates rather than Cartesian

Details

Multiply a coordinate vector in homogeneous coordinates by pre-multiplying by the generated matrix (see examples).

Value

A transformation matrix.

Author(s)

Gert van Valkenhoef

See Also

- `solution.basis`

---

**eliminateRedundant**: Eliminate redundant linear constraints

Description

Given a set of linear constraints, gives a subset of these constraints that are non-redundant.

Usage

eliminateRedundant(constr)

Arguments

- **constr**: Constraints

Details

If no constraints are redundant, returns the same set of constraints.
findExtremePoints

Value

A set of non-redundant constraints.

Author(s)

Gert van Valkenhoef, Tommi Tervonen

See Also

harConstraints

Examples

constr <- list(
  constr = rbind(
    c(-1, 0),
    c(0, 0),
    c(0, 1),
    c(0, 0.5),
  dir = c("<=", "="),
  rhs = c(1))

constr <- eliminateRedundant(constr)

stopifnot(nrow(constr$constr) == 3) # eliminates one constraint

findExtremePoints Find extreme points

Description

Find extreme points of a polytope given by a set of linear constraints along each dimension.

Usage

findExtremePoints(constr, homogeneous=FALSE)

Arguments

constr Constraint definition
homogeneous Whether constr is given in homogeneous coordinate representation

Details

See har for a description of the constraint definition and the homogeneous coordinate representation.

For n-dimensional coordinate vectors, solves 2n LPs to find the extreme points along each dimension.
findFace

Value
A matrix, in which each row is a coordinate vector in the appropriate coordinate system.

Author(s)
Gert van Valkenhoef

See Also
har
findInteriorPoint findVertices
lpccd

Examples
# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("="", ","<=")
constr <- list(constr=A, rhs=b, dir=d)

findExtremePoints(constr, homogeneous=FALSE)

findFace
Find the closest face (constraint) to an interior point of a polytope.

Description
Find the closest face (constraint) to an interior point of a polytope defined by a set of linear constraints.

Usage
findFace(x, constr)

Arguments
x An interior point
constr Constraint definition

Details
See har for a description of the constraint definition.

Value
A face index.
findInteriorPoint

Author(s)
Gert van Valkenhoef

See Also
har

Examples

# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("<=", "<=", "<=")
constr <- list(constr=A, rhs=b, dir=d)

stopifnot(findFace(c(0.1, 0.2), constr) == 1)
stopifnot(findFace(c(0.2, 0.1), constr) == 2)
stopifnot(findFace(c(0.4, 0.4), constr) == 3)

Description
Find an interior point of a polytope given by a set of linear constraints along each dimension.

Usage
findInteriorPoint(constr, homogeneous=FALSE, randomize=FALSE)

Arguments

constr  Constraint definition
homogeneous  Whether constr is given in homogeneous coordinate representation
randomize  Whether the point should be randomized

Details
See har for a description of the constraint definition and the homogeneous coordinate representation.
Solves a slack-maximizing LP to find an interior point of the polytope defined by the given constraints. The randomized version randomly scales the slack on each (non-redundant) constraint.

Value
A vector.
Author(s)
Gert van Valkenhoef

See Also
har
findExtremePoints
findVertices
lpCdd

Examples
# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("=" , ">=" , "<=")
constr <- list(constr=A, rhs=b, dir=d)

findInteriorPoint(constr, homogeneous=FALSE)

findVertices
Find vertices of the polytope

Description
Find the vertices of a polytope given by a set of linear constraints.

Usage
findVertices(constr, homogeneous=FALSE)

Arguments
constr Constraint definition
homogeneous Whether constr is given in homogeneous coordinate representation

Details
See har for a description of the constraint definition and the homogeneous coordinate representation.

Uses the Avis-Fukuda pivoting algorithm to enumerate the vertices of the polytope.

Value
A matrix, in which each row is a vertex of the polytope.

Author(s)
Gert van Valkenhoef
See Also

har
findExtremePoints findInteriorPoint
scdd

Examples

# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("<=", "<=", "<=")
constr <- list(constr=A, rhs=b, dir=d)

findVertices(constr, homogeneous=FALSE)

har "Hit and Run" sampler

Description

The "Hit and Run" method generates a Markov Chain whose stable state converges on the uniform
distribution over a convex polytope defined by a set of linear constraints.

Usage

har(x0, constr, N, thin=1, homogeneous=FALSE, transform=NULL)

Arguments

x0 Starting point (must be in the polytope)
constr Constraint definition (see details)
N Number of iterations to run
thin Thinning factor (keep every \textquoteleft thin\textquoteright-th sample)
homogeneous Whether x0, constr and transform are given in homogeneous coordinate repre-
sentation (see details)
transform Transformation matrix to apply to the generated samples (optional)

Details

The constraints, starting point and transformation matrix can be given in homogeneous coordinate
representation (an extra component is added to each vector, equal to 1.0). This enables affine trans-
formations (such as translation) to be applied to the coordinate vectors by the constraint and trans-
formation matrices. Be aware that while non-affine (perspective) transformations are also possible,
they will not in general preserve uniformity of the generated samples.

Constraints are given as a list(constr=A, rhs=b, dir=d), where d should contain only "<=". See
hitandrun for a "Hit and Run" sampler that also supports equality constraints. The constraints
define the polytope as usual for linear programming: \( Ax \leq b \). In particular, it must be true that
\( Ax_0 \leq b \).
Value

A list, containing:

- **samples**: A matrix containing the generated samples as rows.
- **xN**: The last generated sample, untransformed. Can be used as the starting point for a continuation of the chain.

Note

"Hit and Run" is a Markov Chain Monte Carlo (MCMC) method, so generated samples form a correlated time series. To get a uniform sample, you need $O(n^3)$ samples, where $n$ is the dimension of the sampling space.

Author(s)

Gert van Valkenhoef

References


See Also

harConstraints hitandrun

Examples

```r
# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c(">="", "<="", "<="")
constr <- list(constr=A, rhs=b, dir=d)

# take a point x0 within the polytope
x0 <- c(0.25, 0.25)

# sample 10,000 points
samples <- har(x0, constr, 1E4)$samples

# Check dimension of result
stopifnot(dim(samples) == c(1E4, 2))

# Check that x_i >= 0
stopifnot(samples >= 0)

# Check that x_1 + x_2 <= 1
stopifnot(samples[,1] + samples[,2] <= 1)

plot(samples)
```
Description

These utility functions generate linear constraints

Usage

- `simplexConstraints(n)`
- `lowerBoundConstraint(n, i, x)`
- `upperBoundConstraint(n, i, x)`
- `lowerRatioConstraint(n, i, j, x)`
- `upperRatioConstraint(n, i, j, x)`
- `exactRatioConstraint(n, i, j, x)`
- `ordinalConstraint(n, i, j)`
- `mergeConstraints(...)`

Arguments

- `n` Number of dimensions (vector components)
- `i` Index of first component
- `j` Index of second component
- `x` Scalar bound
- `...` Constraint definitions, or a single list of constraint definitions

Details

See `har` for a description of the constraint format.

- `simplexConstraints` encodes the n-simplex: $\forall k w_k \geq 0$ and $\sum_k w_k = 1$
- `lowerBoundConstraint` encodes $w_i \geq x$
- `upperBoundConstraint` encodes $w_i \leq x$
- `lowerRatioConstraint` encodes $w_i / w_j \geq x$
- `upperRatioConstraint` encodes $w_i / w_j \leq x$
- `exactRatioConstraint` encodes $w_i / w_j = x$
- `ordinalConstraint` encodes $w_i \geq w_j$

`mergeConstraints` merges the constraints it is given. Alternatively, the function takes a single list of constraint definitions which are to be merged.

Value

A constraint definition (concatenation of the given constraint definitions).
hitandrun

"Hit and Run" sampler

Description

The "Hit and Run" method generates a Markov Chain whose stable state converges on the uniform distribution over a convex polytope defined by a set of linear inequality constraints. hitandrun further uses the Moore-Penrose pseudo-inverse to eliminate an arbitrary set of linear equality constraints before applying the "Hit and Run" sampler.

har.init and har.run together provide a re-entrant version of hitandrun so that the Markov chain can be continued if convergence is not satisfactory.
Usage

```r
hitandrun(constr, n.samples=1E4,
         thin.fn = function(n) { ceiling(log(n + 1)/4 * n^3) }, thin = NULL,
         x0.randomize=FALSE, x0.method="slacklp", x0 = NULL, eliminate = TRUE)

har.init(constr,
         thin.fn = function(n) { ceiling(log(n + 1)/4 * n^3) }, thin = NULL,
         x0.randomize=FALSE, x0.method="slacklp", x0 = NULL, eliminate = TRUE)

har.run(state, n.samples)
```

Arguments

- **constr**: Linear constraints that define the sampling space (see details)
- **n.samples**: The desired number of samples to return. The sampler is run for `n.samples * thin` iterations
- **thin.fn**: Function that specifies a thinning factor depending on the dimension of the sampling space after equality constraints have been eliminated. Will only be invoked if `thin` is `NULL`
- **thin**: The thinning factor
- **x0**: Seed point for the Markov Chain. The seed point is specified in the original space, and transformed to the sampling space automatically.
- **x0.method**: Method to generate the seed point if `x0` is unspecified, see `createSeedPoint`
- **x0.randomize**: Whether to generate a random seed point if `x0` is unspecified
- **eliminate**: Whether to eliminate redundant constraints before constructing the transformation to the sampling space and (optionally) calculating the seed point.
- **state**: A state object, as generated by `har.init` (see value)

Details

The constraints are given as a list with the elements `constr`, `dir` and `rhs`. `dir` is a vector with values `"="` or `"<="`. `constr` is a matrix and `rhs` a vector, which encode the standard linear programming constraint froms `Ax = b` and `Ax <= b` (depending on `dir`). The lengths of `rhs` and `dir` must match the number of rows of `constr`.

`hitandrun` applies `solution.basis` to generate a basis of the (translated) solution space of the linear constraints (if any). An affine transformation is generated using `createTransform` and applied to the constraints. Then, a seed point satisfying the inequality constraints is generated using `createSeedPoint`. Finally, `har` is used to generate the samples.

Value

- For `hitandrun`, a matrix containing the generated samples as rows.
- For `har.init`, a state object, containing:
  - **basis**: The basis for the sampling space. See `solution.basis`.
  - **transform**: The sampling space transformation. See `createTransform`. 

The linear inequality constraints translated to the sampling space. See `transformConstraints`.  

The generated seed point. See `createSeedPoint`.  

The thinning factor to be used.

For `har.run`, a list containing:

- `samples` A matrix containing the generated samples as rows.
- `state` A state object that can be used to continue sampling from the Markov chain (i.e. `x0` has been modified).

**Note**

"Hit and Run" is a Markov Chain Monte Carlo (MCMC) method, so generated samples form a correlated time series. To get a uniform sample, you need $O^*(n^3)$ samples, where $n$ is the dimension of the sampling space.

**Author(s)**

Gert van Valkenhoef

**See Also**

- `harConstraints`
- `har`

**Examples**

# Sample from the 3-simplex with the additional constraint that w_1/w_2 = 2  
# Three inequality constraints, two equality constraints  
constr <- mergeConstraints(simplexConstraints(3), exactRatioConstraint(3, 1, 2, 2))  
samples <- hitandrun(constr, n.samples=1000)  
stopifnot(dim(samples) == c(1000, 3))  
stopifnot(all.equal(apply(samples, 1, sum), rep(1, 1000)))  
stopifnot(all.equal(samples[,1]/samples[,2], rep(2, 1000)))

# Sample from the unit rectangle (no equality constraints)  
constr <- list(  
  constr = rbind(c(1,0), c(0,1), c(-1,0), c(0,-1)),  
  dir=rep('<=', 4),  
  rhs=c(1, 1, 0, 0))  
state <- har.init(constr)  
result <- har.run(state, n.samples=1000)  
samples <- result$samples  
stopifnot(all(samples >= 0 & samples <= 1))  
# Continue sampling from the same chain:  
result <- har.run(result$state, n.samples=1000)  
samples <- rbind(samples, result$samples)
**hypersphere.sample**  
*Sample uniformly from an n-hypersphere*

**Description**
Generates uniform random variates over an n-hypersphere

**Usage**

```r
hypersphere.sample(n, N)
```

**Arguments**

- **n**: Dimension of the hypersphere
- **N**: Number of samples

**Value**
A single n-dimensional sample from the hypersphere.

**Author(s)**
Tommi Tervonen <tommi@smaa.fi>

**Examples**
```r
n <- 3 # Dimension
N <- 5 # Nr samples
sample <- hypersphere.sample(n, N)

# Check summing to unity
vec.norm <- function(x) { sum(x^2) }
stopifnot(all.equal(apply(sample, 1, vec.norm), rep(1, N)))
```

---

**sab**  
"Shake and Bake" sampler

**Description**
The "Shake and Bake" method generates a Markov Chain whose stable state converges on the uniform distribution over the boundary of a convex polytope defined by a set of linear constraints.

**Usage**

```r
sab(x0, i0, constr, N, thin=1, homogeneous=FALSE, transform=NULL)
```
Arguments

- **x0**: Starting point (must be in the polytope)
- **i0**: Index of the closest face to the starting point
- **constr**: Constraint definition (see details)
- **N**: Number of iterations to run
- **thin**: Thinning factor (keep every 'thin'-th sample)
- **homogeneous**: Whether x0, constr and transform are given in homogeneous coordinate representation (see details)
- **transform**: Transformation matrix to apply to the generated samples (optional)

Details

The constraints, starting point and transformation matrix can be given in homogeneous coordinate representation (an extra component is added to each vector, equal to 1.0). This enables affine transformations (such as translation) to be applied to the coordinate vectors by the constraint and transformation matrices. Be aware that while non-affine (perspective) transformations are also possible, they will not in general preserve uniformity of the generated samples.

Constraints are given as a list(constr=A, rhs=b, dir=d), where d should contain only "<=". See `shakeandbake` for a "Shake and Bake" sampler that also supports equality constraints. The constraints define the polytope as usual for linear programming: \( Ax \leq b \). In particular, it must be true that \( Ax_0 \leq b \). Points are generated from the boundary of the polytope (where equality holds for one of the constraints), using the "running" shake and bake sampler, which samples the direction vector so that every move point is accepted (Boender et al. 1991).

Value

A list, containing:

- **samples**: A matrix containing the generated samples as rows.
- **faces**: A vector containing the indices of the faces on which the samples lie.
- **xN**: The last generated sample, untransformed. Can be used as the starting point for a continuation of the chain.
- **iN**: Face on which the last generated sample lies.

Note

"Shake and Bake" is a Markov Chain Monte Carlo (MCMC) method, so generated samples form a correlated time series.

Author(s)

Gert van Valkenhoef
shakeandbake

References


See Also

harConstraints shakeandbake

Examples

# constraints: x_1 >= 0, x_2 >= 0, x_1 + x_2 <= 1
A <- rbind(c(-1, 0), c(0, -1), c(1, 1))
b <- c(0, 0, 1)
d <- c("<=", "=")  
constr <- list(constr=A, rhs=b, dir=d)

# take a point x0 within the polytope
x0 <- c(0.25, 0.25)

# sample 10,000 points
result <- sab(x0, 1, constr, 1E4)
samples <- result$samples

# Check dimension of result
stopifnot(dim(samples) == c(1E4, 2))

# Check that x_i >= 0
stopifnot(samples >= -1E-15)

# Check that x_1 + x_2 <= 1
stopifnot(samples[,1] + samples[,2] <= 1 + 1E-15)

# check that the results lie on the faces
faces <- result$faces
stopifnot(all.equal(samples[faces==1,1], rep(0, sum(faces==1))))
stopifnot(all.equal(samples[faces==2,2], rep(0, sum(faces==2))))
stopifnot(all.equal(samples[faces==3,1] + samples[faces==3,2], rep(1, sum(faces==3))))

plot(samples)
Description

The "Shake and Bake" method generates a Markov Chain whose stable state converges on the uniform distribution over a the boundary of a convex polytope defined by a set of linear inequality constraints. *shakeandbake* further uses the Moore-Penrose pseudo-inverse to eliminate an arbitrary set of linear equality constraints before applying the "Shake and Bake" sampler.

`sab.init` and `sab.run` together provide a re-entrant version of `shakeandbake` so that the Markov chain can be continued if convergence is not satisfactory.

Usage

```r
shakeandbake(constr, n.samples=1E4,
    thin.fn = function(n) { ceiling(log(n + 1)/4 * n^3) }, thin = NULL,
    x0.randomize=FALSE, x0.method="slacklp", x0 = NULL, eliminate = TRUE)
```

```r
sab.init(constr,
    thin.fn = function(n) { ceiling(log(n + 1)/4 * n^3) }, thin = NULL,
    x0.randomize=FALSE, x0.method="slacklp", x0 = NULL, eliminate = TRUE)
```

```r
sab.run(state, n.samples)
```

Arguments

- **constr**: Linear constraints that define the sampling space (see details)
- **n.samples**: The desired number of samples to return. The sampler is run for `n.samples * thin` iterations
- **thin.fn**: Function that specifies a thinning factor depending on the dimension of the sampling space after equality constraints have been eliminated. Will only be invoked if `thin` is `NULL`
- **thin**: The thinning factor
- **x0**: Seed point for the Markov Chain. The seed point is specified in the original space, and transformed to the sampling space automatically.
- **x0.method**: Method to generate the seed point if `x0` is unspecified, see `createSeedPoint`
- **x0.randomize**: Whether to generate a random seed point if `x0` is unspecified
- **eliminate**: Whether to eliminate redundant constraints before constructing the transformation to the sampling space and (optionally) calculating the seed point.
- **state**: A state object, as generated by `har.init` (see value)

Details

The constraints are given as a list with the elements `constr`, `dir` and `rhs`. `dir` is a vector with values `'='` or `'<='`. `constr` is a matrix and `rhs` a vector, which encode the standard linear programming constraint froms `Ax = b` and `Ax \leq b` (depending on `dir`). The lengths of `rhs` and `dir` must match the number of rows of `constr`.

`shakeandbake` applies `solution.basis` to generate a basis of the (translated) solution space of the linear constraints (if any). An affine transformation is generated using `createTransform` and
applied to the constraints. Then, a seed point satisfying the inequality constraints is generated using `createSeedPoint`. The closest face to this point is found using `findFace`. Finally, `sab` is used to generate the samples.

Value

For `shakeandbake`, a matrix containing the generated samples as rows.
For `sab.init`, a state object, containing:

- **basis**: The basis for the sampling space. See `solution.basis`.
- **transform**: The sampling space transformation. See `createTransform`.
- **constr**: The linear inequality constraints translated to the sampling space. See `transformConstraints`.
- **x0**: The generated seed point. See `createSeedPoint`.
- **i0**: The index of the closest face. See `findFace`.
- **thin**: The thinning factor to be used.

For `sab.run`, a list containing:

- **samples**: A matrix containing the generated samples as rows.
- **state**: A state object that can be used to continue sampling from the Markov chain (i.e. `x0` and `i0` have been modified).

Note

"Shake and Bake" is a Markov Chain Monte Carlo (MCMC) method, so generated samples form a correlated time series.

Author(s)

Gert van Valkenhoef

See Also

- `harConstraints` `sab`

Examples

```r
# Sample from the 3-simplex with the additional constraint that w_1/w_2 = 2
# Three inequality constraints, two equality constraints
constr <- mergeConstraints(simplexConstraints(3), exactRatioConstraint(3, 1, 2, 2))
samples <- shakeandbake(constr, n.samples=1000)
stopifnot(dim(samples) == c(1000, 3))
stopifnot(all.equal(apply(samples, 1, sum), rep(1, 1000)))

sel <- samples[,3] > 0.5 # detect which side we're on
stopifnot(all.equal(samples[sel,], matrix(rep(c(0,0,1), each=sum(sel)), ncol=3)))
stopifnot(all.equal(samples[!sel,], matrix(rep(c(2/3,1/3,0), each=sum(sel)), ncol=3)))

# Sample from the unit rectangle (no equality constraints)
constr <- list(
```
constr = rbind(c(1,0), c(0,1), c(-1,0), c(0,-1)),
dir=rep('<=', 4),
rhs=c(1, 1, 0, 0))
state <- sab.init(constr)
result <- sab.run(state, n.samples=1000)
faces <- result$faces
samples <- result$samples
stopifnot(all(samples >= -1e-15 & samples <= 1 + 1e-15))

stopifnot(all.equal(samples[faces==1,1], rep(1, sum(faces==1))))
stopifnot(all.equal(samples[faces==2,2], rep(1, sum(faces==2))))
stopifnot(all.equal(samples[faces==3,1], rep(0, sum(faces==3))))
stopifnot(all.equal(samples[faces==4,2], rep(0, sum(faces==4))))

# Continue sampling from the same chain:
result <- sab.run(result$state, n.samples=1000)
samples <- rbind(samples, result$samples)

---

**simplex.createConstraints**

Create constraints that define the (n-1)-simplex

**Description**

This function takes a transformation matrix from the plane coincident with the (n-1) simplex and (optionally) additional constraints defined in n-dimensional space, and generates a set of constraints defining the simplex and (optionally) the additional constraints in the (n-1)-dimensional homogeneous coordinate system.

**Usage**

```r
simplex.createConstraints(transform, userConstr=NULL)
```

**Arguments**

- `transform` Transformation matrix
- `userConstr` Additional constraints

**Details**

The transformation of the constraint matrix to (n-1)-dimensional homogeneous coordinates is a necessary preprocessing step for applying "Hit and Run" to subsets of the simplex defined by `userConstr`.

**Value**

A set of constraints in the (n-1)-dimensional homogeneous coordinate system.
**simplex.createTransform**

Transform points on an (n-1)-simplex to n-dimensional space

**Description**

This function generates a matrix to transform points in an (n-1) dimensional homogeneous coordinate representation of the (n-1) simplex to n-dimensional Cartesian coordinates.

The inverse transform can also be generated, and conversion can be to homogeneous coordinates instead of Cartesian ones.

**Author(s)**

Gert van Valkenhoef

**See Also**

`simplex.createTransform` `har` `harConstraints`

**Examples**

```r
n <- 3
userConstr <- mergeConstraints(
  ordinalConstraint(3, 1, 2), ordinalConstraint(3, 2, 3))

transform <- simplex.createTransform(n)
constr <- simplex.createConstraints(transform, userConstr)
seedPoint <- createSeedPoint(constr, homogeneous=TRUE)

N <- 10000
samples <- har(seedPoint, constr, N, 1, homogeneous=TRUE, transform=transform)$samples

# Check dimension
stopifnot(dim(samples) == c(N, n))

# Check that w_i >= w_i+1
stopifnot(sapply(1:(n-1), function(i) {
  all(samples[,i]>=samples[,i+1])
}))

# Check that w_i >= 0
stopifnot(samples >= 0)

# Check that sum_i w_i = 1
E <- 1E-12
stopifnot(apply(samples, 1, sum) > 1 - E)
stopifnot(apply(samples, 1, sum) < 1 + E)
```
Usage

```r
simplex.createTransform(n, inverse=FALSE, keepHomogeneous=inverse)
```

Arguments

- `n` Dimension of the space
- `inverse` TRUE to convert from n-space coordinates to (n-1)-simplex coordinates
- `keepHomogeneous` TRUE to convert to homogeneous coordinates rather than Cartesian

Details

Multiply a coordinate vector in homogeneous coordinates by pre-multiplying by the generated matrix (see examples).

Value

A transformation matrix.

Author(s)

Gert van Valkenhoef

See Also

- `simplex.createConstraints`
- `har`

Examples

```r
E <- 1E-12 # Allowed numerical error

# The origin in (n-1)-dimensional space should be the centroid of the simplex
# when transformed to n-dimensional space
transform <- simplex.createTransform(3)
x <- transform %*% c(0, 0, 1)
x
stopifnot(abs(x - c(1/3, 1/3, 1/3)) < E)

# The same should hold for the inverse transformation
invTransform <- simplex.createTransform(3, inverse=TRUE)
y <- invTransform %*% c(1/3, 1/3, 1/3, 1)
y
stopifnot(abs(y - c(0, 0, 1)) < E)

# Of course, an arbitrary weight vector should transform back to itself
transform <- simplex.createTransform(3, keepHomogeneous=TRUE)
x <- c(0.2, 0.5, 0.3, 1.0)
y <- transform %*% invTransform %*% x
y
stopifnot(abs(y - x) < E)
```
# And we can apply the transform to a matrix:
a <- cbind(x, x, x)
b <- transform %*% invTransform %*% a
stopifnot(abs(b - a) < E)

simplex.sample Sample uniformly from a simplex

Description

Generates uniform random variates over the (n-1)-simplex in n-dimensional space.

Usage

simplex.sample(n, N, sort=FALSE)

Arguments

n Dimension of the space
N Number of samples to generate
sort Whether to sort the components in descending order

Details

The samples will be uniform over the (n-1)-simplex.

Value

samples A matrix containing the generated samples as rows.

Author(s)

Gert van Valkenhoef

Examples

n <- 3
N <- 10000
samples <- simplex.sample(n, N)$samples

# Check dimension
stopifnot(dim(samples) == c(N, n))

# Check that w_i >= 0
stopifnot(samples >= 0)

# Check that sum_i w_i = 1
E <- 1E-12

# Check that sum_i w_i = 1
```r
stopifnot(apply(samples, 1, sum) > 1 - E)
stopifnot(apply(samples, 1, sum) < 1 + E)

## Now with descending order
samples <- simplex.sample(n, N, sort=TRUE)$samples

# Check dimension
stopifnot(dim(samples) == c(N, n))

# Check that w_i >= 0
stopifnot(samples >= 0)

# Check that sum_i w_i = 1
E <- 1E-12
stopifnot(apply(samples, 1, sum) > 1 - E)
stopifnot(apply(samples, 1, sum) < 1 + E)

# Check w_i >= w_{i+1}
stopifnot(samples[,1] >= samples[,2])
stopifnot(samples[,2] >= samples[,3])
```

---

**solution.basis**

*Calculate the basis for the solution space of a system of linear equations*

---

**Description**

Given a set of linear equality constraints, determine a translation and a basis for its solution space.

**Usage**

`solution.basis(constr)`

**Arguments**

- `constr` Linear equality constraints

**Details**

For a system of linear equations, $Ax = b$, the solution space is given by

$$x = A^\dagger b + (I - A^\dagger A)y$$

where $A^\dagger$ is the Moore-Penrose pseudoinverse of $A$. The QR decomposition of $I - A^\dagger A$ enables us to determine the dimension of the solution space and derive a basis for that space.
transformConstraints

Value
A list, consisting of

- **translate** A point in the solution space
- **basis** A basis rooted in that point

Author(s)
Gert van Valkenhoef

See Also
createTransform

Examples

```r
# A 3-dimensional original space
n <- 3

# x_1 + x_2 + x_3 = 1
eq.constr <- list(constr = t(rep(1, n)), dir = '=', rhs = 1)
basis <- solution.basis(eq.constr)
stopifnot(ncol(basis$basis) == 2) # Dimension reduced to 2
y <- rbind(rnorm(100, 0, 100), rnorm(100, 0, 100))
x <- basis$basis %*% y + basis$translate
stopifnot(all.equal(apply(x, 2, sum), rep(1, 100)))

# 2 x_2 = x_1; 2 x_3 = x_2
eq.constr <- mergeConstraints(
  eq.constr,
  list(constr = c(-1, 2, 0), dir = '=', rhs = 0),
  list(constr = c(0, -1, 2), dir = '=', rhs = 0))
basis <- solution.basis(eq.constr)
stopifnot(ncol(basis$basis) == 0) # Dimension reduced to 0
stopifnot(all.equal(basis$translate, c(4/7, 2/7, 1/7)))
```

---

transformConstraints Apply a transformation to a set of linear constraints.

Description
Given a set of linear constraints and a transformation matrix, return the constraints in the transformed space.

Usage

```r
transformConstraints(transform, constr)
```
Transforming the constraint matrix is a necessary preprocessing step for applying "Hit and Run" to subsets of a space defined by linear equality constraints. See `solution.basis` and `createTransform` for building the transformation matrix.

**Value**

A set of constraints in the new basis.

**Author(s)**

Gert van Valkenhoef

**See Also**

`solution.basis` `createTransform` `har`

**Examples**

```r
# Sample from the space where 2*x_1 = x_2 + x_3 and
# 0 <= x_1, x_2, x_3 <= 5
n <- 3
eq.constr <- list(
  constr = matrix(c(2, -1, -1), nrow=1, ncol=n),
  dir = '=',
  rhs = 0)
ineq.constr <- list(
  constr = rbind(-diag(n), diag(n)),
  dir = rep('<=', n * 2),
  rhs = c(rep(0, n), rep(5, n)))

basis <- solution.basis(eq.constr)
transform <- createTransform(basis)
constr <- transformConstraints(transform, ineq.constr)
x0 <- createSeedPoint(constr, homogeneous=TRUE)
x <- har(x0, constr, 500, transform=transform, homogeneous=TRUE)$samples

stopifnot(all.equal(2 * x[,1], x[,2] + x[,3]))
stopifnot(all(x >= 0))
stopifnot(all(x <= 5))
```
Index

* bounding box
  bbReject, 4
  createBoundBox, 5

* constraint
  eliminateRedundant, 8
  harConstraints, 15
  simplex.createConstraints, 24
  transformConstraints, 29

* hit-and-run
  har, 13
  harConstraints, 15
  hitandrun, 16
  hitandrun-package, 2

* hypersphere
  hypersphere.sample, 19

* seed point
  createSeedPoint, 6
  findExtremePoints, 9
  findInteriorPoint, 11
  findVertices, 12

* shake-and-bake
  sab, 19
  shakeandbake, 21

* simplex
  simplex.createConstraints, 24
  simplex.createTransform, 25
  simplex.sample, 27

* transform
  createTransform, 7
  simplex.createTransform, 25
  solution.basis, 28
  transformConstraints, 29

* uniform sampling
  bbReject, 4
  har, 13
  hitandrun, 16
  hypersphere.sample, 19
  sab, 19
  shakeandbake, 21

  simplex.sample, 27

  bbReject, 2, 3, 4
  createBoundBox, 3, 4, 5
  createSeedPoint, 3, 6, 17, 18, 22, 23
  createTransform, 2, 3, 7, 17, 22, 23, 29, 30
  eliminateRedundant, 8, 16
  exactRatioConstraint (harConstraints), 15
  findExtremePoints, 5–7, 9, 12, 13
  findFace, 10, 23
  findInteriorPoint, 10, 11, 13
  findVertices, 7, 10, 12, 12
  har, 2–7, 9–13, 13, 15–18, 25, 26, 30
  har.init (hitandrun), 16
  har.run (hitandrun), 16
  harConstraints, 2–4, 9, 14, 15, 18, 21, 23, 25
  hitandrun, 2, 3, 13, 14, 16, 16
  hitandrun-package, 2
  hypersphere.sample, 3, 19
  lowerBoundConstraint (harConstraints), 15
  lowerRatioConstraint (harConstraints), 15
  lpcdd, 10, 12
  mergeConstraints (harConstraints), 15
  ordinalConstraint (harConstraints), 15
  sab, 2, 19, 23
  sab.init (shakeandbake), 21
  sab.run (shakeandbake), 21
  scdd, 13
  shakeandbake, 2, 20, 21, 21
  simplex.createConstraints, 2–4, 24, 26
simplex.createTransform, 2–4, 25, 25
simplex.sample, 2, 3, 27
simplexConstraints (harConstraints), 15
solution.basis, 2, 3, 8, 17, 22, 23, 28, 30
transformConstraints, 2, 3, 18, 23, 29
upperBoundConstraint (harConstraints), 15
upperRatioConstraint (harConstraints), 15