

Package ‘vdg’

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Description Facilities for constructing variance dispersion graphs, fraction-of-design-space plots and similar graphics for exploring the properties of experimental designs. The design region is explored via random sampling, which allows for more flexibility than traditional variance dispersion graphs. A formula interface is leveraged to provide access to complex model formulae. Graphics can be constructed simultaneously for multiple experimental designs and/or multiple model formulae. Instead of using pointwise optimization to find the minimum and maximum scaled prediction variance curves, which can be inaccurate and time consuming, this package uses quantile regression as an alternative.

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Contents

vdg-package	2
D310	3
D416B	3
D416C	4
GJ54	4
LHS	5
meanspv	6
plot.spv	7
print.spv	11
runif_cube	12
sampler	13
SCDDL5	14
SCDH5	15
spv	15
stdrange	18
Index	19

vdg-package	<i>Variance Dispersion Graphs, Fraction-of-Design-Space Plots and Variants</i>
-------------	--

Description

This package provides functionality for producing variance dispersion graphs (VDGs), fraction-of-design (FDS) plots and related graphics for assessing the prediction variance properties of experimental designs. Random sampling is used to assess the distribution of the prediction variance throughout the design region. Multiple design and/or model formulae can be assessed at the same time. Graphics are produced by the **ggplot2** package.

Details

The workhorse function in the package is `spv`, which takes lists of experimental designs and / or model formulae and produces samples throughout the design region at which the prediction variance is evaluated. Depending on the type of input for the design and formula arguments, `spv` creates output objects of S3 classes `spv`, `spvlist`, `spvforlist` or `spvlistforlist`. The graphical output are obtained with the `plot` methods of these classes, and the `which` argument can be used to control the type of plots produced.

The design regions allowed for are typically spherical or cuboidal in nature, but the `keepfun` argument to `spv` can be used for rejection sampling. In this way nonstandard design regions can be allowed for. See also the `type` argument of `spv`. The output from the `plot` methods for objects created by `spv` are typically named lists of graphical objects created by **ggplot2**. These are best stored in an object and recreated by printing the required plot. Storing such graphical objects also enables post-hoc manipulation of the plots, such as changing the background colour by using **ggplot2**'s `theme` function.

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The vdg Package. *Journal of Statistical Software*, 74(3), 1-22. doi:[10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

See Also

[spv](#), [plot.spv](#), and `vignette(topic = "vdg")`.

D310

Design from the Vdgraph package

Description

This data frame is taken verbatim from the (now archived) **Vdgraph** package. See that package for the original reference.

Usage

D310

Format

a data frame of 10 runs in three variables.

References

Lawson J, Vining G (2014). *Vdgraph: Variance dispersion graphs and Fraction of design space plots for response surface designs*. R package version 2.2-2, <https://CRAN.R-project.org/package=Vdgraph>.

D416B

Design from the Vdgraph package

Description

This data frame is taken verbatim from the (now archived) **Vdgraph** package. See that package for the original reference.

Usage

D416B

Format

a data frame of 16 runs in four variables.

References

Lawson J, Vining G (2014). *Vdgraph: Variance dispersion graphs and Fraction of design space plots for response surface designs*. R package version 2.2-2, <https://CRAN.R-project.org/package=Vdgraph>.

D416C

Design from the Vdgraph package

Description

This data frame is taken verbatim from the (now archived) **Vdgraph** package. See that package for the original reference.

Usage

D416C

Format

a data frame of 16 runs in four variables.

References

Lawson J, Vining G (2014). *Vdgraph: Variance dispersion graphs and Fraction of design space plots for response surface designs*. R package version 2.2-2, <https://CRAN.R-project.org/package=Vdgraph>.

GJ54

Design from Goos & Jones

Description

This data frame contains the design of Table 5.4 in Goos & Jones (2011).

Usage

GJ54

Format

a data frame of 15 runs in two variables: Time (seconds) and Temperature (Kelvin)

References

Goos, P., & Jones, B. (2011). *Optimal design of experiments: a case study approach*. John Wiley & Sons.

LHS*Latin Hypercube Sampling*

Description

Different versions of latin hypercube sampling (LHS): ordinary LHS, midpoint LHS, symmetric LHS or randomized symmetric LHS. LHS is a method for constructing space-filling designs. They can be more efficient for hypercuboidal design regions than other sampling methods.

Usage

```
LHS(n, m = 3, lim = c(-1, 1))  
MLHS(n, m = 3, lim = c(-1, 1))  
SLHS(n, m = 3, lim = c(-1, 1))  
RSLHS(n, m = 3, lim = c(-1, 1))
```

Arguments

n	number of design points to generate
m	number of design factors
lim	limits of the coordinates in all dimensions

Value

Matrix with samples as rows.

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The vdg Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

Examples

```
set.seed(1234)  
pts <- seq(-1, 1, length = 11)  
  
# Ordinary LHS  
samp <- LHS(n = 10, m = 2)  
plot(samp, main = "LHS")  
abline(h = pts, v = pts, col = "lightgrey")
```

```

# Midpoint LHS
samp <- MLHS(n = 10, m = 2)
plot(samp, main = "MLHS")
abline(h = pts, v = pts, col = "lightgrey")

# Symmetric LHS
samp <- SLHS(n = 10, m = 2)
plot(samp, main = "SLHS")
abline(h = pts, v = pts, col = "lightgrey")

# Randomized Symmetric LHS
samp <- RSLHS(n = 10, m = 2)
plot(samp, main = "RSLHS")
abline(h = pts, v = pts, col = "lightgrey")

```

meanspv

*Compute Mean Spherical SPV***Description**

Computes the matrix of spherical region moments for a given model formula and a vector of radii, and uses this to calculate the mean spherical SPV for each of the radii. The function `expmat` calculates the matrix containing the exponents of each model factor within each model term as columns. Only simple formulae are allowed for. Only products of terms should be included in calls to `I`. The power operator `^` should be used instead of `sqrt`. Models should contain only monomial terms.

Usage

```

meanspv(formula, radii, FtF.inv, n)

expmat(formula)

```

Arguments

<code>formula</code>	model formula
<code>radii</code>	numeric vector or radii at which to calculate the matrix of spherical region moments
<code>FtF.inv</code>	inverse of $F'F$, where F is the design matrix
<code>n</code>	integer giving the number of design runs

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The vdg Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

Examples

```
f1 <- formula(~ x1*x2)
expmat(f1)
f2 <- update(f1, ~ . + I(x1^2) + I(x2^2))
expmat(f2)
f3 <- update(f2, ~ . + I(x2^0.4))
expmat(f3)
f4 <- update(f3, ~ . + I(x1^2):I(x2^2))
expmat(f4)
f5 <- update(f4, ~ . + I(x1^3*x2^0.5))
expmat(f5)
```

plot.spv

Plot VDGs or FDS plots

Description

Produce Variance Dispersion Graphs and/or Fraction of Design Space plots for experimental designs. There are methods for the S3 classes spv, spvlist, spvforlist and spvlistforlist – see [spv](#).

Usage

```
## S3 method for class 'spv'
plot(
  x,
  which = c("fds", "vdgsim", "vdgquantile", "vdgboth", "boxplots"),
  np = 50,
  alpha = 7/sqrt(length(x$spv)),
  points.colour = "#39BEB1",
  points.size = 2,
  tau = c(0.05, 0.95),
  radii = 21,
  hexbin = FALSE,
  bins = 80,
  df = 10,
  lines.size = 1,
  origin = rep(0, ncol(x$sample)),
  method,
  arrange = FALSE,
  ...
)
```

```

)

## S3 method for class 'spvforlist'
plot(
  x,
  which = c("fds", "vdgsim", "vdgquantile", "vdgboth", "boxplots"),
  np = 50,
  alpha = 7/sqrt(length(x[[1]]$spv)),
  points.colour = "#39BEB1",
  points.size = 2,
  tau = c(0.05, 0.95),
  radii = 21,
  hexbin = FALSE,
  bins = 80,
  df = 10,
  lines.size = 1,
  origin = rep(0, ncol(x[[1]]$sample)),
  method,
  arrange = FALSE,
  ...
)

## S3 method for class 'spvlist'
plot(
  x,
  which = c("fds", "vdgsim", "vdgquantile", "vdgboth", "boxplots"),
  np = 50,
  alpha = 7/sqrt(length(x[[1]]$spv)),
  points.colour = "#39BEB1",
  points.size = 2,
  tau = c(0.05, 0.95),
  radii = 21,
  hexbin = FALSE,
  bins = 80,
  VRFDS = FALSE,
  df = 10,
  lines.size = 1,
  origin = rep(0, ncol(x[[1]]$sample)),
  method,
  arrange = FALSE,
  ...
)

## S3 method for class 'spvlistforlist'
plot(
  x,
  which = c("fds", "vdgsim", "vdgquantile", "vdgboth", "boxplots"),
  np = 50,

```



```

alpha = 7/sqrt(length(x[[1]][[1]]$spv)),
points.colour = "#39BEB1",
points.size = 2,
tau = c(0.05, 0.95),
radii = 21,
hexbin = FALSE,
bins = 80,
df = 10,
lines.size = 1,
origin = rep(0, ncol(x[[1]][[1]]$sample)),
method,
arrange = FALSE,
...
)

```

Arguments

<code>x</code>	an object of type <code>spv</code> for a single experimental design or an object of type <code>spvlist</code> for multiple designs.
<code>which</code>	either a numeric vector of integers or a character vector indicating which plots to produce. The possible plots are: 1 or <code>"fds"</code> A (variance ratio) FDS plot 2 or <code>"vdgsim"</code> A VDG with only the simulated prediction variance points plotted 3 or <code>"vdgquantile"</code> A VDG with only the quantile regression lines corresponding to <code>tau</code> shown 4 or <code>"vdgboth"</code> A combination of 2 and 3 5 or <code>"boxplots"</code> Parallel boxplots of the prediction variance
<code>np</code>	scalar; the number of points to use for calculating the fraction of design space criterion.
<code>alpha</code>	the alpha transparency coefficient for the plots
<code>points.colour</code>	colour for points in scatterplot of SPV against the radius
<code>points.size</code>	size for points in scatterplot of SPV against the radius
<code>tau</code>	the tau parameter for <code>rq</code> (quantile regression)
<code>radii</code>	either a numeric vector containing the radii to use for calculating the mean spherical SPV over the spherical design space, or an integer (length one vector) giving the number of radii to use for calculating the mean spherical SPV. If missing, the mean spherical SPV is not used.
<code>hexbin</code>	logical indicating whether hexagonal binning should be used to display density instead of colour transparency
<code>bins</code>	argument passed to <code>stat_binhex</code> to determine the number of hexagons used for binning.
<code>df</code>	degrees-of-freedom parameter passed to <code>bs</code>
<code>lines.size</code>	line size passed to <code>geom_line</code>

origin	numeric vector specifying the origin of the design space
method	optional; passed to <code>dist</code> to overwrite defaults of "Euclidean" for spherical regions or "supremum" for cuboidal regions
arrange	Logical indicating whether to return a single graphical object arranging the resulting plots in a single plot window via <code>grid.arrange</code> , or whether to return the list of graphical objects containing the plots.
...	additional arguments passed to <code>dist</code>
VRFDS	logical indicating whether to construct a variance ratio FDS plot or not (only for class <code>spvlist</code>). The first design is used as reference design in case of VRFDS is TRUE

Value

Returns a list of `ggplot` graphical objects (or grobs) with names corresponding to the character version of which. These plot objects can be manipulated by changing plot aesthetics and theme elements.

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The `vdg` Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

Examples

```
# Single design (class 'spv')
# Larger n should be used in actual cases
library(rsm)
bbd3 <- as.data.frame(bbd(3)[,3:5])
colnames(bbd3) <- paste0("x", 1:3)
quad.3f <- formula(~ x1*x2*x3 - x1:x2:x3 + I(x1^2) + I(x2^2) + I(x3^2))
set.seed(1234)
out <- spv(n = 1000, design = bbd3, type = "spherical", formula = quad.3f)
out
plot(out)

# List of designs (class 'spvlist')
## Not run:
data(SCDH5); data(SCDDL5)
des.list <- list(SCDH5 = SCDH5, SCDDL5 = SCDDL5)
quad.5f <- formula(~ x1 + x2 + x3 + x4 + x5 + x1:x2 + x1:x3 + x1:x4 + x1:x5
+ x2:x3 + x2:x4 + x2:x5 + x3:x4 + x3:x5 + x4:x5
+ I(x1^2) + I(x2^2) + I(x3^2) + I(x4^2) + I(x5^2))
out2 <- spv(n = 500, design = des.list, type = "spherical", formula = quad.5f)
out2
plot(out2)
```

```
## End(Not run)

# List of formulae (class 'spvforlist')
## Not run:
fact3 <- expand.grid(x1 = c(-1,1), x2 = c(-1, 1), x3 = c(-1,1))
lin.3f <- formula(~ x1 + x2 + x3)
int.3f <- formula(~ (x1+x2+x3)^2)
set.seed(4312)
out3 <- spv(n = 500, design = fact3, type = "cuboidal",
            formula = list(linear = lin.3f, interaction = int.3f))
out3
plot(out3)

## End(Not run)

# List of formulae and designs (class 'spvlistforlist')
## Not run:
fact3.n <- rbind(fact3, 0, 0, 0)
set.seed(4312)
out4 <- spv(n = 200, design = list(factorial = fact3, factorial.with.cnt = fact3.n),
            type = "cuboidal", formula = list(linear = lin.3f, interaction = int.3f))
out4
plot(out4)

## End(Not run)
```

print.spv

Print Method for S3 spv classes

Description

Simple print methods for S3 classes `spv`, `spvlist`, `spvforlist` and `spvlistforlist`. See [plot.spv](#) for examples.

Usage

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

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

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

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

Arguments

x	Object of class spv or spvlist
...	Unimplemented

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The vdg Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

runif_cube	<i>Sampling for hyperspheres/hypercubes</i>
------------	---

Description

Sample uniformly in or on a hyperspheres or hypercubes.

Usage

```
runif_cube(n, m = 2, max.dist = 1, at = FALSE, nr.dist = 21)
runif_sphere(n, m = 2, max.radius = sqrt(m), at = FALSE, nr.rad = 21)
```

Arguments

n	number of points to sample
m	number of design factors
max.dist	maximum distance from origin (L-infinity norm/supremum distance) for the hypercuboidal design region (enveloping hypercube)
at	logical indicating whether to sample on concentric hyperspheres/hypercubes or not. With this option n is distributed proportionally across radii / supremum distances so that the density of samples on each concentric hypercube / hypersphere are uniform across the different hyperspheres / hypercubes..
nr.dist	the number of concentric hypercubes to use in case at is TRUE
max.radius	maximum radius of the hyperspherical design region (enveloping hypersphere)
nr.rad	number of concentric hyperspheres to sample on in case of at being TRUE

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The *vdg* Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

Examples

```
set.seed(1234)
runif_sphere(n = 10)

set.seed(1234)
samp <- runif_sphere(n = 500, at = TRUE)
plot(samp, asp = 1)
```

sampler	<i>Sampler Function</i>
---------	-------------------------

Description

This is a wrapper for the sampling functions of the **vdg** package. It extracts design properties from the design passed to it to take appropriate samples.

Usage

```
sampler(
  n,
  design,
  type = c("spherical", "cuboidal", "lhs", "mlhs", "slhs", "rslhs", "custom"),
  at = FALSE,
  custom.fun = NULL,
  ...
)
```

Arguments

n	number of points to sample
design	design for which the sample is required (either a matrix or data frame)
type	type of design region/sampling method. One of "spherical", "cuboidal", "lhs", "mlhs", "slhs", "rslhs" or "custom". Option "custom" requires custom.fun to be non-NULL.
at	logical; should sampling be done on the surface of hyperspheres or hypercubes? Not used for LHS methods.
custom.fun	A custom sampling function, used in conjunction with type = "custom". The first and second arguments must be the sample size and dimension respectively.
...	other arguments passed to the underlying sampling functions.

Value

Matrix with samples as rows, with S3 class `smp1`

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The `vdg` Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

See Also

[runif_sphere](#), [runif_cube](#), [LHS](#), [MLHS](#), [SLHS](#), [RSLHS](#)

Examples

```
## Default spherical design region
set.seed(1896)
smp1 <- sampler(n = 100, design = expand.grid(x = -1:1, y = -1:1))
plot(smp1)

## Supplying a custom sampling function based on lhs::improvedLHS()
library("lhs")
sfun <- function(n, k, dup = 1) 2 * improvedLHS(n, k, dup = dup) - 1
smp2 <- sampler(n = 100, design = expand.grid(x = -1:1, y = -1:1),
               type = "custom", custom.fun = sfun)
plot(smp2)
```

SCDDL5

Design from the Vdgraph package

Description

This data frame is taken verbatim from the (now archived) **Vdgraph** package. See that package for the original reference.

Usage

SCDDL5

Format

a data frame of 23 runs in five variables.

References

Lawson J, Vining G (2014). *Vdgraph: Variance dispersion graphs and Fraction of design space plots for response surface designs*. R package version 2.2-2, <https://CRAN.R-project.org/package=Vdgraph>.

SCDH5	<i>Design from the Vdgraph package</i>
-------	--

Description

This data frame is taken verbatim from the (now archived) **Vdgraph** package. See that package for the original reference.

Usage

SCDH5

Format

a data frame of 28 runs in four variables.

References

Lawson J, Vining G (2014). *Vdgraph: Variance dispersion graphs and Fraction of design space plots for response surface designs*. R package version 2.2-2, <https://CRAN.R-project.org/package=Vdgraph>.

spv	<i>Calculate the Scaled Prediction Variance (or SPV)</i>
-----	--

Description

Calculates the SPV for a sample of points in a design region of specified type. Sampling is done by calling [sampler](#).

Usage

```
spv(
  n,
  design,
  type = "spherical",
  formula,
  at = FALSE,
  keepfun,
  sample,
```

```

    unscaled = FALSE,
    ...
)

## S3 method for class 'data.frame'
spv(
  n,
  design,
  type = c("spherical", "cuboidal", "lhs", "mlhs", "slhs", "rslhs", "custom"),
  formula,
  at = FALSE,
  keepfun,
  sample,
  unscaled = FALSE,
  ...
)

## S3 method for class 'list'
spv(
  n,
  design,
  type = c("spherical", "cuboidal", "lhs", "mlhs", "slhs", "rslhs", "custom"),
  formula,
  at = FALSE,
  keepfun,
  sample,
  unscaled = FALSE,
  ...
)

## S3 method for class 'matrix'
spv(
  n,
  design,
  type = c("spherical", "cuboidal", "lhs", "mlhs", "slhs", "rslhs", "custom"),
  formula,
  at = FALSE,
  keepfun,
  sample,
  unscaled = FALSE,
  ...
)

```

Arguments

n	number of samples to take
design	a design or list of designs. Each design must be either a matrix or a data.frame or coercible to a data.frame.

type	type of sampling passed to sampler
formula	either a single model formula or a list of formulae
at	only used when type is 'spherical' or 'cuboidal'
keepfun	optional; function operating on the columns of a matrix with the same number of columns as design which return a logical value for including a specific point in the sample or not. Useful for rejection sampling for nonstandard design regions.
sample	optional; if not missing it should contain a matrix or data.frame containing points sampled over the required design region. If it is not missing, no further sampling will be done: the SPV is simply evaluated at these points.
unscaled	logical indicating whether to use the unscaled prediction variance (UPV) instead of the scale prediction variance (SPV)
...	additional arguments passed to sampler . This enables the use of user-specified sampling functions via the custom.fun argument to sampler .

Value

Object of class 'spv', 'spvlist', 'spvforlist' or 'spvlistforlist', depending on whether single designs/formulas are passed or lists of these.

Author(s)

Pieter C. Schoonees

References

Pieter C. Schoonees, Niel J. le Roux, Roelof L.J. Coetzer (2016). Flexible Graphical Assessment of Experimental Designs in R: The vdg Package. *Journal of Statistical Software*, 74(3), 1-22. [doi:10.18637/jss.v074.i03](https://doi.org/10.18637/jss.v074.i03).

See Also

[plot.spv](#) for more examples

Examples

```
# Single design (class 'spv')
library(rsm)
bbd3 <- as.data.frame(bbd(3)[,3:5])
colnames(bbd3) <- paste0("x", 1:3)
quad.3f <- formula(~(x1 + x2 + x3)^2 - x1:x2:x3)
out <- spv(n = 1000, design = bbd3, type = "spherical", formula = quad.3f)
out
```

stdrange	<i>Standardize or Unstandarize the Column Range</i>
----------	---

Description

Simple functions for rescaling a data matrix to a coded design and back. `stdrange` converts the design in actual measurements into a coded design, while `ustdrange` reverses the process (if the correct arguments are given).

Usage

```
stdrange(x, mins = apply(x, 2, min), maxs = apply(x, 2, max))
```

```
ustdrange(x, mins, maxs)
```

Arguments

<code>x</code>	matrix containing the design, or an object coercible to a matrix.
<code>mins</code>	vector of original values, one for each column, which should be recoded to the value -1; or which have already been recoded to -1. This and the next argument are both recycled if not of the correct length.
<code>maxs</code>	vector of original values which should be recoded as 1, or which have already been recoded to 1.

Author(s)

Pieter C. Schoonees

Index

- * **design**
 - LHS, [5](#)
- * **hplot**
 - plot.spv, [7](#)
- * **multivariate**
 - spv, [15](#)
- * **package**
 - vdg-package, [2](#)
- * **print**
 - print.spv, [11](#)
- [^](#), [6](#)
- [bs](#), [9](#)
- [D310](#), [3](#)
- [D416B](#), [3](#)
- [D416C](#), [4](#)
- [dist](#), [10](#)
- [expmat \(meanspv\)](#), [6](#)
- [geom_line](#), [9](#)
- [ggplot](#), [10](#)
- [GJ54](#), [4](#)
- [grid.arrange](#), [10](#)
- [I](#), [6](#)
- [LHS](#), [5](#), [14](#)
- [meanspv](#), [6](#)
- [MLHS](#), [14](#)
- [MLHS \(LHS\)](#), [5](#)
- [plot](#), [2](#)
- [plot.spv](#), [3](#), [7](#), [11](#), [17](#)
- [plot.spvforlist \(plot.spv\)](#), [7](#)
- [plot.spvlist \(plot.spv\)](#), [7](#)
- [plot.spvlistforlist \(plot.spv\)](#), [7](#)
- [print.spv](#), [11](#)
- [print.spvforlist \(print.spv\)](#), [11](#)
- [print.spvlist \(print.spv\)](#), [11](#)
- [print.spvlistforlist \(print.spv\)](#), [11](#)
- [rq](#), [9](#)
- [RSLHS](#), [14](#)
- [RSLHS \(LHS\)](#), [5](#)
- [runif_cube](#), [12](#), [14](#)
- [runif_sphere](#), [14](#)
- [runif_sphere \(runif_cube\)](#), [12](#)
- [sampler](#), [13](#), [15](#), [17](#)
- [SCDDL5](#), [14](#)
- [SCDH5](#), [15](#)
- [SLHS](#), [14](#)
- [SLHS \(LHS\)](#), [5](#)
- [spv](#), [2](#), [3](#), [7](#), [15](#)
- [sqrt](#), [6](#)
- [stat_binhex](#), [9](#)
- [stdrange](#), [18](#)
- [theme](#), [2](#)
- [ustdrange \(stdrange\)](#), [18](#)
- [vdg-package](#), [2](#)