

Package ‘GDSARM’

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Title Gauss - Dantzig Selector: Aggregation over Random Models

Version 0.1.1

Description The method aims to identify important factors in screening experiments by aggregation over random models as studied in Singh and Stufken (2022) <[doi:10.48550/arXiv.2205.13497](https://doi.org/10.48550/arXiv.2205.13497)>. This package provides functions to run the Gauss-Dantzig selector on screening experiments when interactions may be affecting the response. Currently, all functions require each factor to be at two levels coded as +1 and -1.

License GPL (>= 3)

Encoding UTF-8

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URL <https://github.com/agrakhi/GDSARM>

BugReports <https://github.com/agrakhi/GDSARM/issues>

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dantzig.delta	<i>Dantzig selector with an option to make profile plot</i>
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Description

The Dantzig selector (DS) finds a solution for the model parameters of a linear model, β using linear programming. For a given δ , DS minimizes the L_1 -norm (sum of absolute values) of β subject to the constraint that $\max(|t(X)(y - X * \beta)|) \leq \delta$.

Usage

```
dantzig.delta(X, y, delta, plot = FALSE)
```

Arguments

X	a design matrix.
y	a vector of responses.
delta	a vector with the values of δ for which the DS optimization needs to be solved.
plot	a boolean value of either TRUE or FALSE with TRUE indicating that the profile plot should be drawn.

Value

A matrix of the estimated values of β with each row corresponding to a particular value of δ .

Source

Candès, E. and Tao, T. (2007). The Dantzig selector: Statistical estimation when p is much larger than n . *Annals of Statistics* 35 (6), 2313–2351.

Phoa, F. K., Pan, Y. H. and Xu, H. (2009). Analysis of supersaturated designs via the Dantzig selector. *Journal of Statistical Planning and Inference* 139 (7), 2362–2372.

See Also

[GDS_givencols](#), [GDSARM](#)

Examples

```
data(dataHamadaWu)
X = dataHamadaWu[,-8]
Y = dataHamadaWu[,8]
#scale and center X and y
scaleX = base::scale(X, center= TRUE, scale = TRUE)
scaleY = base::scale(Y, center= TRUE, scale = FALSE)
```

```
maxDelta = max(abs(t(scaleX)%*%matrix(scaleY, ncol=1)))
# Dantzig Selector on 4 equally spaced delta values between 0 and maxDelta
dantzig.delta(scaleX, scaleY, delta = seq(0,maxDelta,length.out=4))
```

dataCompoundExt

Compound Extraction experiment of Dopico-García et al. (2007)

Description

An analytical experiment conducted by Dopico-García et al. (2007) to characterize the chemical composition of white grapes simultaneously determining the most important phenolic compounds and organic acids for the grapes. This example has been further studied in Phoa et al. (2009b) for one phenolic compound, kaempferol-3-Orutinoside + isorhamnetin-3-O glucoside, which is also what we studied. It is accepted for these data that fitting a main-effects model suggests that V3 (Factor C), V4 (Factor D), and interaction V1:V4 (A:D) are active effects.

Usage

```
data(dataCompoundExt)
```

Format

A data frame with 12 rows and 9 columns:

V1 Factor A

V2 Factor B

V3 Factor C

V4 Factor D

V5 Factor E

V6 Factor F

V7 Factor G

V8 Factor H

V9 Response

Source

Dopico-García, M.S., Valentao, P., Guerra, L., Andrade, P. B., and Seabra, R. M. (2007). Experimental design for extraction and quantification of phenolic compounds and organic acids in white "Vinho Verde" grapes *Analytica Chimica Acta*, 583(1): 15–22.

Phoa, F. K., Wong, W. K., and Xu, H (2009b). The need of considering the interactions in the analysis of screening designs. *Journal of Chemometrics: A Journal of the Chemometrics Society*, 23(10): 545–553.

Examples

```
data(dataCompoundExt)
X = dataCompoundExt[,-9]
Y= dataCompoundExt[,9]
```

dataHamadaWu

Cast fatigue experiment of Hunter et al. (1982)

Description

A cast fatigue experiment with 12 runs and 7 factors was originally studied by Hunter et al. (1982), and was later revisited by Hamada and Wu (1992) and Phoa et al. (2009), among others. It is widely accepted for these data that V6 (F) and interaction V6:V7 (F:G) are active effects, with interaction of V1:V5 (A:E) possibly being active as well.

Usage

```
data(dataHamadaWu)
```

Format

A data frame with 12 rows and 8 columns:

- V1** Factor A
- V2** Factor B
- V3** Factor C
- V4** Factor D
- V5** Factor E
- V6** Factor F
- V7** Factor G
- V8** Response

Source

Hamada, M. and C. F. J. Wu (1992). Analysis of designed experiments with complex aliasing. *Journal of Quality Technology* 24 (3), 130–137.

Hunter, G. B., F. S. Hodi, and T. W. Eagar (1982). High cycle fatigue of weld repaired cast Ti-6Al-4V. *Metallurgical Transactions A* 13 (9), 1589–1594.

Phoa, F. K., Y. H. Pan, and H. Xu (2009). Analysis of supersaturated designs via the Dantzig selector. *Journal of Statistical Planning and Inference* 139 (7), 2362–2372.

Examples

```
data(dataHamadaWu)
X = dataHamadaWu[,-8]
Y= dataHamadaWu[,8]
```

GDSARM *Gauss-Dantzig Selector - Aggregation over Random Models (GDS-ARM)*

Description

The GDS-ARM procedure consists of three steps. First, it runs the Gauss Dantzig Selector (GDS) `nrep` times, each time with a different set of `nint` randomly selected two-factor interactions. All `m` main effects are included in each GDS run. Second, the best `ntop` models are identified with the smallest BIC. Effects that appear in at least `pkeep` \times `ntop` of the `ntop` models are then passed on to the third stage. In the third stage, stepwise regression is used. With `n` being the number of runs, the stepwise regression starts with at most `n-3` selected effects from the previous step. The remaining effects from the previous step as well as all main effects are given a chance to enter into the model using the forward-backward stepwise regression. The function also has the option of using the modified GDS-ARM. The modified version incorporates effect heredity in two steps, first, for each model found by GDS, we ignore active interactions when at least one of the main effects is not active (for weak heredity) or when both main effects are not active (for strong heredity); and second, we do the same for the model found after the stepwise stage of GDS-ARM.

Usage

```
GDSARM(
  delta.n = 10,
  nint,
  nrep,
  ntop,
  pkeep,
  design,
  Y,
  cri.penter = 0.01,
  cri.premove = 0.05,
  opt.heredity = c("none"),
  seedvalue = 1234
)
```

Arguments

<code>delta.n</code>	a positive integer suggesting the number of delta values to be tried. <code>delta.n</code> equally spaced values of <code>delta</code> will be used strictly between 0 and $\max(t(X)y)$. The default value is set to 10.
<code>nint</code>	a positive integer representing the number of randomly chosen interactions. The suggested value to use is the ceiling of 20% of the total number of interactions, that is, for <code>m</code> factors, we have $\text{ceiling}(0.2(m \text{ choose } 2))$.
<code>nrep</code>	a positive integer representing the number of times GDS should be run. The suggested value is $(m \text{ choose } 2)$.

<code>ntop</code>	a positive integer representing the number of top models to be selected among the <code>nrep</code> models. The suggested value is $\max(20, (\text{nrep} \times \text{nint}) / (m(m-1)))$. The value of <code>ntop</code> should not exceed <code>nrep</code> .
<code>pkeep</code>	a number between 0 and 1 representing the proportion of <code>ntop</code> models in which an effect needs to appear in order to be selected for the stepwise regression stage.
<code>design</code>	a $n \times m$ matrix of <code>m</code> two-level factors. The levels should be coded as +1 and -1.
<code>Y</code>	a vector of <code>n</code> responses.
<code>cri.penter</code>	the p-value cutoff for the most significant effect to enter into the stepwise regression model. The suggested value is 0.01.
<code>cri.remove</code>	the p-value cutoff for the least significant effect to exit from the stepwise regression model. The suggested value is 0.05.
<code>opt.heredity</code>	a string with either none, or weak, or strong. Denotes whether the effect-heredity (weak or strong) should be embedded in GDS-ARM. The default value is none as suggested in Singh and Stufken (2022).
<code>seedvalue</code>	a seed value that will fix the set of interactions being selected. The default value is seed to 1234.

Value

A list returning the selected effects as well as the corresponding important factors.

Source

Candes, E. and Tao, T. (2007). The Dantzig selector: Statistical estimation when p is much larger than n . *Annals of Statistics* 35 (6), 2313–2351.

Dopico-García, M.S., Valentao, P., Guerra, L., Andrade, P. B., and Seabra, R. M. (2007). Experimental design for extraction and quantification of phenolic compounds and organic acids in white "Vinho Verde" grapes *Analytica Chimica Acta*, 583(1): 15–22.

Hamada, M. and Wu, C. F. J. (1992). Analysis of designed experiments with complex aliasing. *Journal of Quality Technology* 24 (3), 130–137.

Hunter, G. B., Hodi, F. S. and Eagar, T. W. (1982). High cycle fatigue of weld repaired cast Ti-6Al-4V. *Metallurgical Transactions A* 13 (9), 1589–1594.

Phoa, F. K., Pan, Y. H. and Xu, H. (2009). Analysis of supersaturated designs via the Dantzig selector. *Journal of Statistical Planning and Inference* 139 (7), 2362–2372.

Singh, R. and Stufken, J. (2022). Factor selection in screening experiments by aggregation over random models, 1–31. doi: [10.48550/arXiv.2205.13497](https://doi.org/10.48550/arXiv.2205.13497)

See Also

[GDS_givencols](#), [dantzig.delta](#)

Examples

```

data(dataHamadaWu)
X = dataHamadaWu[,-8]
Y = dataHamadaWu[,8]
delta.n = 10
n = dim(X)[1]
m = dim(X)[2]
nint = ceiling(0.2*choose(m,2))
nrep = choose(m,2)
ntop = max(20, nint*nrep/(2*choose(m,2)))
pkeep = 0.25
cri.penter = 0.01
cri.premove = 0.05
design = X
# GDS-ARM with default values
GDSARM(delta.n, nint, nrep, ntop, pkeep, X, Y, cri.penter, cri.premove)

# GDS-ARM with default values but with weak heredity
opt.heredity="weak"
GDSARM(delta.n, nint, nrep, ntop, pkeep, X, Y, cri.penter, cri.premove, opt.heredity)

data(dataCompoundExt)
X = dataCompoundExt[,-9]
Y = dataCompoundExt[,9]
delta.n = 10
n = dim(X)[1]
m = dim(X)[2]
nint = ceiling(0.2*choose(m,2))
nrep = choose(m,2)
ntop = max(20, nint*nrep/(2*choose(m,2)))
pkeep = 0.25
cri.penter = 0.01
cri.premove = 0.05
design = X
# GDS-ARM on compound extraction
GDSARM(delta.n, nint, nrep, ntop, pkeep, X, Y, cri.penter, cri.premove)

# GDS-ARM on compound extraction with strong heredity
opt.heredity = "strong"
GDSARM(delta.n, nint, nrep, ntop, pkeep, X, Y, cri.penter, cri.premove, opt.heredity)

```

GDS_givencols

Gauss-Dantzig Selector

Description

This function runs the Gauss-Dantzig selector on the given columns. We have two options: either (a) GDS(m) on the m main effects, and (b) GDS($m+2f$) on the m main effects and the corresponding

two-factor interactions. For a given `delta`, DS minimizes the L₁-norm (sum of absolute values) of `beta` subject to the constraint that $\max(|t(X)(y-X * beta)|) \leq \text{delta}$. The GDS is run for multiple values of `delta`. We use `kmeans` and `BIC` to select a best model.

Usage

```
GDS_givencols(delta.n = 10, design, Y, which.cols = c("main2fi"))
```

Arguments

<code>delta.n</code>	a positive integer suggesting the number of <code>delta</code> values to be tried. <code>delta.n</code> equally spaced values of <code>delta</code> will be used strictly between 0 and $\max(t(X)y)$. The default value is set to 10.
<code>design</code>	a $n \times m$ matrix of <code>m</code> two-level factors. The levels should be coded as +1 and -1.
<code>Y</code>	a vector of <code>n</code> responses.
<code>which.cols</code>	a string with either <code>main</code> or <code>main2fi</code> . Denotes whether the Gauss-Dantzig Selector should be run on the main effect columns (<code>main</code>), or on all main effects plus all 2 factor interaction columns (<code>main2fi</code>). The default value is <code>main2fi</code> .

Value

A list returning the selected effects as well as the corresponding important factors.

Source

Candes, E. and Tao, T. (2007). The Dantzig selector: Statistical estimation when p is much larger than n . *Annals of Statistics* 35 (6), 2313–2351.

Dopico-García, M.S., Valente, P., Guerra, L., Andrade, P. B., and Seabra, R. M. (2007). Experimental design for extraction and quantification of phenolic compounds and organic acids in white "Vinho Verde" grapes *Analytica Chimica Acta*, 583(1): 15–22.

Hamada, M. and Wu, C. F. J. (1992). Analysis of designed experiments with complex aliasing. *Journal of Quality Technology* 24 (3), 130–137.

Hunter, G. B., Hodi, F. S. and Eagar, T. W. (1982). High cycle fatigue of weld repaired cast Ti-6Al-4V. *Metallurgical Transactions A* 13 (9), 1589–1594.

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Singh, R. and Stufken, J. (2022). Factor selection in screening experiments by aggregation over random models, 1–31. doi: [10.48550/arXiv.2205.13497](https://doi.org/10.48550/arXiv.2205.13497)

See Also

[GDSARM](#), [dantzig.delta](#)

Examples

```
data(dataHamadaWu)
X = dataHamadaWu[,-8]
Y = dataHamadaWu[,8]
delta.n = 10
# GDS on main effects
GDS_givencols(delta.n, design = X, Y=Y, which.cols = "main")

# GDS on main effects and two-factor interactions
GDS_givencols(delta.n, design = X, Y=Y)

data(dataCompoundExt)
X = dataCompoundExt[,-9]
Y = dataCompoundExt[,9]
delta.n = 10
# GDS on main effects
GDS_givencols(delta.n, design = X, Y=Y, which.cols = "main")
# GDS on main effects and two-factor interactions
GDS_givencols(delta.n, design = X, Y=Y, which.cols = "main2fi")
```

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