

Package ‘grasps’

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Type Package

Title Groupwise Regularized Adaptive Sparse Precision Solution

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Description Provides a unified framework for sparse-group regularization and precision matrix estimation in Gaussian graphical models. It implements multiple sparse-group penalties, including sparse-group lasso, sparse-group adaptive lasso, sparse-group SCAD, and sparse-group MCP, and solves them efficiently using ADMM-based optimization. The package is designed for high-dimensional network inference where both sparsity and group structure are present.

License GPL (>= 3)

URL <https://github.com/Carol-seven/grasps>,
<https://shiyong-xiao.com/grasps/>

BugReports <https://github.com/Carol-seven/grasps/issues>

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compute_derivative	<i>Penalty Derivative Computation</i>
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Description

Compute one or more derivative values for a given omega, allowing vectorized specifications of penalty, lambda, and gamma.

Usage

```
compute_derivative(omega, penalty, lambda, gamma = NA)
```

Arguments

omega	A numeric value or vector at which the penalty is evaluated.
penalty	A character string or vector specifying one or more penalty types. Available options include: 1. "lasso": Least absolute shrinkage and selection operator (Tibshirani 1996; Friedman et al. 2008). 2. "atan": Arctangent type penalty (Wang and Zhu 2016). 3. "exp": Exponential type penalty (Wang et al. 2018). 4. "lq": Lq penalty (Frank and Friedman 1993; Fu 1998; Fan and Li 2001). 5. "lsp": Log-sum penalty (Candès et al. 2008). 6. "mcp": Minimax concave penalty (Zhang 2010). 7. "scad": Smoothly clipped absolute deviation (Fan and Li 2001; Fan et al. 2009). If penalty has length 1, it is recycled to the common length determined by penalty, lambda, and gamma.
lambda	A non-negative numeric value or vector specifying the regularization parameter. If lambda has length 1, it is recycled to the common length determined by penalty, lambda, and gamma.

gamma A numeric value or vector specifying the additional parameter for the penalty function. If **lambda** has length 1, it is recycled to the common length determined by **penalty**, **lambda**, and **gamma**. The penalty-specific defaults are:

1. "atan": 0.005
2. "exp": 0.01
3. "lq": 0.5
4. "lsp": 0.1
5. "mcp": 3
6. "scad": 3.7

For "lasso", **gamma** is ignored.

Value

A data frame with S3 class "derivative" containing:

omega The input omega values.

penalty The penalty type for each row.

lambda The regularization parameter used.

gamma The additional penalty parameter used.

value The computed derivative value.

The number of rows equals $\max(\text{length}(\text{penalty}), \text{length}(\text{lambda}), \text{length}(\text{gamma}))$. Any of **penalty**, **lambda**, or **gamma** with length 1 is recycled to this common length.

References

- Candès EJ, Wakin MB, Boyd SP (2008). "Enhancing Sparsity by Reweighted ℓ_1 Minimization." *Journal of Fourier Analysis and Applications*, **14**(5), 877–905. doi:10.1007/s000410089045x.
- Fan J, Feng Y, Wu Y (2009). "Network Exploration via the Adaptive LASSO and SCAD Penalties." *The Annals of Applied Statistics*, **3**(2), 521–541. doi:10.1214/08aoas215.
- Fan J, Li R (2001). "Variable Selection via Nonconcave Penalized Likelihood and its Oracle Properties." *Journal of the American Statistical Association*, **96**(456), 1348–1360. doi:10.1198/016214501753382273.
- Frank LE, Friedman JH (1993). "A Statistical View of Some Chemometrics Regression Tools." *Technometrics*, **35**(2), 109–135. doi:10.1080/00401706.1993.10485033.
- Friedman J, Hastie T, Tibshirani R (2008). "Sparse Inverse Covariance Estimation with the Graphical Lasso." *Biostatistics*, **9**(3), 432–441. doi:10.1093/biostatistics/kxm045.
- Fu WJ (1998). "Penalized Regressions: The Bridge versus the Lasso." *Journal of Computational and Graphical Statistics*, **7**(3), 397–416. doi:10.1080/10618600.1998.10474784.
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Wang Y, Fan Q, Zhu L (2018). “Variable Selection and Estimation using a Continuous Approximation to the L_0 Penalty.” *Annals of the Institute of Statistical Mathematics*, **70**(1), 191–214. doi:10.1007/s1046301605883.

Wang Y, Zhu L (2016). “Variable Selection and Parameter Estimation with the Atan Regularization Method.” *Journal of Probability and Statistics*, **2016**, 6495417. doi:10.1155/2016/6495417.

Zhang C (2010). “Nearly Unbiased Variable Selection under Minimax Concave Penalty.” *The Annals of Statistics*, **38**(2), 894–942. doi:10.1214/09AOS729.

Examples

```
library(grasps)
library(ggplot2)

deriv_df <- compute_derivative(
  omega = seq(0, 4, by = 0.01),
  penalty = c("atan", "exp", "lasso", "lq", "lsp", "mcp", "scad"),
  lambda = 1)

plot(deriv_df) +
  scale_y_continuous(limits = c(0, 1.5)) +
  guides(color = guide_legend(nrow = 2, byrow = TRUE))
```

compute_penalty	<i>Penalty Function Computation</i>
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Description

Compute one or more penalty values for a given omega, allowing vectorized specifications of penalty, lambda, and gamma.

Usage

```
compute_penalty(omega, penalty, lambda, gamma = NA)
```

Arguments

omega	A numeric value or vector at which the penalty is evaluated.
penalty	A character string or vector specifying one or more penalty types. Available options include: 1. "lasso": Least absolute shrinkage and selection operator (Tibshirani 1996; Friedman et al. 2008). 2. "atan": Arctangent type penalty (Wang and Zhu 2016). 3. "exp": Exponential type penalty (Wang et al. 2018). 4. "lq": Lq penalty (Frank and Friedman 1993; Fu 1998; Fan and Li 2001).

5. "lsp": Log-sum penalty (Candès et al. 2008).
6. "mcp": Minimax concave penalty (Zhang 2010).
7. "scad": Smoothly clipped absolute deviation (Fan and Li 2001; Fan et al. 2009).

If penalty has length 1, it is recycled to the common length determined by penalty, lambda, and gamma.

lambda A non-negative numeric value or vector specifying the regularization parameter. If lambda has length 1, it is recycled to the common length determined by penalty, lambda, and gamma.

gamma A numeric value or vector specifying the additional parameter for the penalty function. If lambda has length 1, it is recycled to the common length determined by penalty, lambda, and gamma. The penalty-specific defaults are:

1. "atan": 0.005
2. "exp": 0.01
3. "lq": 0.5
4. "lsp": 0.1
5. "mcp": 3
6. "scad": 3.7

For "lasso", gamma is ignored.

Value

A data frame with S3 class "penalty" containing:

omega The input omega values.

penalty The penalty type for each row.

lambda The regularization parameter used.

gamma The additional penalty parameter used.

value The computed penalty value.

The number of rows equals $\max(\text{length}(\text{penalty}), \text{length}(\text{lambda}), \text{length}(\text{gamma}))$. Any of penalty, lambda, or gamma with length 1 is recycled to this common length.

References

Candès EJ, Wakin MB, Boyd SP (2008). "Enhancing Sparsity by Reweighted ℓ_1 Minimization." *Journal of Fourier Analysis and Applications*, **14**(5), 877–905. doi:10.1007/s000410089045x.

Fan J, Feng Y, Wu Y (2009). "Network Exploration via the Adaptive LASSO and SCAD Penalties." *The Annals of Applied Statistics*, **3**(2), 521–541. doi:10.1214/08aoas215.

Fan J, Li R (2001). "Variable Selection via Nonconcave Penalized Likelihood and its Oracle Properties." *Journal of the American Statistical Association*, **96**(456), 1348–1360. doi:10.1198/016214501753382273.

Frank LE, Friedman JH (1993). "A Statistical View of Some Chemometrics Regression Tools."

Technometrics, **35**(2), 109–135. doi:[10.1080/00401706.1993.10485033](https://doi.org/10.1080/00401706.1993.10485033).

Friedman J, Hastie T, Tibshirani R (2008). “Sparse Inverse Covariance Estimation with the Graphical Lasso.” *Biostatistics*, **9**(3), 432–441. doi:[10.1093/biostatistics/kxm045](https://doi.org/10.1093/biostatistics/kxm045).

Fu WJ (1998). “Penalized Regressions: The Bridge versus the Lasso.” *Journal of Computational and Graphical Statistics*, **7**(3), 397–416. doi:[10.1080/10618600.1998.10474784](https://doi.org/10.1080/10618600.1998.10474784).

Tibshirani R (1996). “Regression Shrinkage and Selection via the Lasso.” *Journal of the Royal Statistical Society: Series B (Methodological)*, **58**(1), 267–288. doi:[10.1111/j.25176161.1996.tb02080.x](https://doi.org/10.1111/j.25176161.1996.tb02080.x).

Wang Y, Fan Q, Zhu L (2018). “Variable Selection and Estimation using a Continuous Approximation to the L_0 Penalty.” *Annals of the Institute of Statistical Mathematics*, **70**(1), 191–214. doi:[10.1007/s1046301605883](https://doi.org/10.1007/s1046301605883).

Wang Y, Zhu L (2016). “Variable Selection and Parameter Estimation with the Atan Regularization Method.” *Journal of Probability and Statistics*, **2016**, 6495417. doi:[10.1155/2016/6495417](https://doi.org/10.1155/2016/6495417).

Zhang C (2010). “Nearly Unbiased Variable Selection under Minimax Concave Penalty.” *The Annals of Statistics*, **38**(2), 894–942. doi:[10.1214/09AOS729](https://doi.org/10.1214/09AOS729).

Examples

```
library(grasps)
library(ggplot2)

pen_df <- compute_penalty(
  omega = seq(-4, 4, by = 0.01),
  penalty = c("atan", "exp", "lasso", "lq", "lsp", "mcp", "scad"),
  lambda = 1)

plot(pen_df, xlim = c(-1, 1), ylim = c(0, 1), zoom.size = 1) +
  guides(color = guide_legend(nrow = 2, byrow = TRUE))
```

gen_prec_sbm

Block-Structured Precision Matrix based on SBM

Description

Generate a precision matrix that exhibits block structure induced by a stochastic block model (SBM).

Usage

```
gen_prec_sbm(
  p,
  block.sizes = NULL,
  K = 3,
```

```

prob.mat = NULL,
within.prob = 0.25,
between.prob = 0.05,
weight.mat = NULL,
weight.dists = list("gamma", "unif"),
weight.paras = list(c(shape = 100, rate = 10), c(min = 0, max = 5)),
cond.target = 100
)

```

Arguments

<code>p</code>	An integer specifying the number of variables (dimensions).
<code>block.sizes</code>	An integer vector (default = NULL) specifying the size of each group. If NULL, the p variables are divided as evenly as possible across K groups.
<code>K</code>	An integer (default = 3) specifying the number of groups. Ignored if <code>block.sizes</code> is provided; then <code>K <- length(block.sizes)</code> .
<code>prob.mat</code>	A $K \times K$ symmetric matrix (default = NULL) specifying the Bernoulli rates. Element (i, j) gives the probability of creating an edge between vertices from groups i and j . If NULL, a matrix with <code>within.prob</code> on the diagonal and <code>between.prob</code> on the off-diagonal is used.
<code>within.prob</code>	A numeric value in $[0, 1]$ (default = 0.25) specifying the probability of creating an edge between vertices within the same group. This argument is used only when <code>prob.mat</code> = NULL.
<code>between.prob</code>	A numeric value in $[0, 1]$ (default = 0.05) specifying the probability of creating an edge between vertices from different groups. This argument is used only when <code>prob.mat</code> = NULL.
<code>weight.mat</code>	A $p \times p$ symmetric matrix (default = NULL) specifying the edge weights. If NULL, weights are generated block-wise according to <code>weight.dists</code> and <code>weight.paras</code> .
<code>weight.dists</code>	A list (default = <code>list("gamma", "unif")</code>) specifying the sampling distribution for each block of weights. Its length determines how the distributions are assigned:

- `length = 1`: Same specification for all blocks.
- `length = 2`: First for within-group blocks, second for between-group blocks.
- `length =  $K + K(K - 1)/2$` : Full specification for each block. The first K elements correspond to within-group blocks with indices $1, \dots, K$, and the remaining $K(K - 1)/2$ elements correspond to between-group blocks ordered as $(1, 2), (1, 3), (1, 4), \dots, (1, K), (2, 3), \dots, (K - 1, K)$.

Each element of `weight.dists` can be:

1. A user-supplied sampling function. The function must accept an argument `n` specifying the number of samples.
2. A character string specifying the distribution family. Accepted distributions (base R samplers in parentheses) include:
 - "beta": Beta distribution ([rbeta](#))
 - "cauchy": Cauchy distribution ([rcauchy](#)).
 - "chisq": Chi-squared distribution ([rchisq](#)).

	• "exp": Exponential distribution (<code>rexp</code>). • "f": F distribution (<code>rf</code>). • "gamma": Gamma distribution (<code>rgamma</code>). • "lnorm": Log normal distribution (<code>rlnorm</code>). • "norm": Normal distribution (<code>rnorm</code>). • "t": Student's t distribution (<code>rt</code>). • "unif": Uniform distribution (<code>runif</code>). • "weibull": Weibull distribution (<code>rweibull</code>).
<code>weight.paras</code>	A list (default = <code>list(c(shape = 100, rate = 10), c(min = 0, max = 5))</code>) specifying the parameters associated with <code>weight.dists</code> . It must follow the same length rules as <code>weight.dists</code> . Each element should be a named vector or list suitable for the corresponding sampler.
<code>cond.target</code>	A numeric value > 1 (default = 100) specifying the target condition number for the precision matrix. When necessary, a diagonal shift is applied to ensure positive definiteness and numerical stability.

Details

Edge sampling. Within- and between-group edges are sampled independently according to Bernoulli distributions specified by `prob.mat`, or by `within.prob` and `between.prob` if `prob.mat` is not supplied.

Weight sampling. Conditional on the adjacency structure, edge weights are sampled block-wise from samplers specified in `weight.dists` and `weight.paras`. The length of `weight.dists` (and `weight.paras`) determines how weight distributions are assigned:

- `length = 1`: Same specification for all blocks.
- `length = 2`: first for within-group blocks, second for between-group blocks.
- `length =  $K + K(K - 1)/2$` : Full specification for each block.

Block indexing. The order for blocks is:

- Within-group blocks: Indices $1, \dots, K$.
- Between-group blocks: $K(K - 1)/2$ blocks in order $(1, 2), (1, 3), (1, 4), \dots, (1, K), (2, 3), \dots, (K - 1, K)$.

Positive definiteness. Motivated by condition-number-regularized covariance estimation (Won et al. 2013), the weighted adjacency matrix is symmetrized and used as the precision matrix Ω_0 . Since arbitrary block-structured weights may not be positive definite, a diagonal adjustment is applied to control the eigenvalue spectrum. Specifically, let $\lambda_{\max}$ and $\lambda_{\min}$ denote the largest and smallest eigenvalues of a matrix. A non-negative numeric value τ is added to the diagonal so that

$$\begin{cases} \frac{\lambda_{\max}(\Omega_0 + \tau I)}{\lambda_{\min}(\Omega_0 + \tau I)} \leq \text{cond.target} \\ \lambda_{\min}(\Omega_0 + \tau I) > 0 \\ \tau \geq 0 \end{cases}$$

which ensures both positive definiteness and guarantees that the condition number does not exceed `cond.target`, providing numerical stability even in high-dimensional settings.

Value

An object with S3 class "gen_prec_sbm" containing the following components:

Omega The precision matrix with SBM block structure.

Sigma The covariance matrix, i.e., the inverse of Omega.

sparsity Proportion of zero entries in Omega.

membership An integer vector specifying the group membership.

References

Won J, Lim J, Kim S, Rajaratnam B (2013). "Condition-Number-Regularized Covariance Estimation." *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **75**(3), 427–450. [doi:10.1111/j.14679868.2012.01049.x](https://doi.org/10.1111/j.14679868.2012.01049.x).

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
#### case 1: base R distribution
sim1 <- gen_prec_sbm(p = 100, K = 5,
                    within.prob = 0.25, between.prob = 0.1,
                    weight.dists = list("gamma", "unif"),
                    weight.paras = list(c(shape = 100, scale = 1e2),
                                       c(min = 0, max = 10)),
                    cond.target = 100)

#### visualization
plot(sim1)

#### case 2: user-defined sampler
my_gamma <- function(n) {
  rgamma(n, shape = 1e4, scale = 1e2)
}
sim2 <- gen_prec_sbm(p = 100, K = 5,
                    within.prob = 0.2, between.prob = 0.05,
                    weight.dists = list(my_gamma, "unif"),
                    weight.paras = list(NULL,
                                       c(min = 0, max = 1)),
                    cond.target = 100)

#### visualization
plot(sim2)
```

grasps

*Groupwise Regularized Adaptive Sparse Precision Solution***Description**

Provide a collection of statistical methods that incorporate both element-wise and group-wise penalties to estimate a precision matrix.

Usage

```
grasps(
  X,
  n = nrow(X),
  membership,
  penalty,
  diag.ind = TRUE,
  diag.grp = TRUE,
  diag.include = FALSE,
  lambda = NULL,
  alpha = NULL,
  gamma = NULL,
  nlambda = 10,
  lambda.min.ratio = 0.01,
  growiter.lambda = 30,
  tol.lambda = 0.001,
  maxiter.lambda = 50,
  rho = 2,
  tau.incr = 2,
  tau.decr = 2,
  nu = 10,
  tol.abs = 1e-04,
  tol.rel = 1e-04,
  maxiter = 10000,
  crit = "BIC",
  kfold = 5,
  ebic.tuning = 0.5
)
```

Arguments

- | | |
|------------|---|
| X | <ol style="list-style-type: none"> 1. An $n \times p$ data matrix with sample size n and dimension p. 2. A $p \times p$ sample covariance matrix with dimension p. |
| n | An integer (default = <code>nrow(X)</code>) specifying the sample size. This is only required when the input matrix X is a $p \times p$ sample covariance matrix with dimension p . |
| membership | An integer vector specifying the group membership. The length of membership must be consistent with the dimension p . |

penalty	A character string specifying the penalty for estimating precision matrix. Available options include: 1. "lasso": Least absolute shrinkage and selection operator (Tibshirani 1996; Friedman et al. 2008). 2. "adapt": Adaptive lasso (Zou 2006; Fan et al. 2009). 3. "atan": Arctangent type penalty (Wang and Zhu 2016). 4. "exp": Exponential type penalty (Wang et al. 2018). 5. "lq": Lq penalty (Frank and Friedman 1993; Fu 1998; Fan and Li 2001). 6. "lsp": Log-sum penalty (Candès et al. 2008). 7. "mcp": Minimax concave penalty (Zhang 2010). 8. "scad": Smoothly clipped absolute deviation (Fan and Li 2001; Fan et al. 2009).
diag.ind	A logical value (default = TRUE) specifying whether to penalize the diagonal elements.
diag.grp	A logical value (default = TRUE) specifying whether to penalize the within-group blocks.
diag.include	A logical value (default = FALSE) specifying whether to include the diagonal entries in the penalty for within-group blocks when <code>diag.grp = TRUE</code> .
lambda	A positive numeric vector specifying the grid for the regularization parameter. The default is NULL, which generates its own lambda sequence based on <code>nlambda</code> and <code>lambda.min.ratio</code> .
alpha	A numeric vector in [0,1] specifying the grid for the mixing parameter balancing the element-wise individual L1 penalty and the block-wise group L2 penalty. An alpha of 1 corresponds to the individual penalty only; an alpha of 0 corresponds to the group penalty only. The default value is a sequence from 0.1 to 0.9 with increments of 0.1. When both alpha and lambda are supplied, all Cartesian combinations of their values are evaluated.
gamma	A numeric value specifying the additional parameter for the chosen penalty. The default value depends on the penalty: 1. "adapt": 0.5 2. "atan": 0.005 3. "exp": 0.01 4. "lq": 0.5 5. "lsp": 0.1 6. "mcp": 3 7. "scad": 3.7
nlambda	An integer (default = 10) specifying the number of lambda values to generate when <code>lambda = NULL</code> .
lambda.min.ratio	A numeric value > 0 (default = 0.01) specifying the fraction of the maximum lambda value $\lambda_{\max}$ to generate the minimum lambda $\lambda_{\min}$. If <code>lambda = NULL</code> , a lambda grid of length <code>nlambda</code> is automatically generated on a log scale, ranging from $\lambda_{\max}$ down to $\lambda_{\min}$.

<code>growiter.lambda</code>	An integer (default = 30) specifying the maximum number of exponential growth steps during the initial search for an admissible upper bound $\lambda_{\max}$.
<code>tol.lambda</code>	A numeric value > 0 (default = 1e-03) specifying the relative tolerance for the bisection stopping rule on the interval width.
<code>maxiter.lambda</code>	An integer (default = 50) specifying the maximum number of bisection iterations in the line search for $\lambda_{\max}$.
<code>rho</code>	A numeric value > 0 (default = 2) specifying the ADMM augmented-Lagrangian penalty parameter (often called the ADMM step size). Larger values typically put more weight on enforcing the consensus constraints at each iteration; smaller values yield more conservative updates.
<code>tau.incr</code>	A numeric value > 1 (default = 2) specifying the multiplicative factor used to increase rho when the primal residual dominates the dual residual in ADMM.
<code>tau.decr</code>	A numeric value > 1 (default = 2) specifying the multiplicative factor used to decrease rho when the dual residual dominates the primal residual in ADMM.
<code>nu</code>	A numeric value > 1 (default = 10) controlling how aggressively rho is rescaled in the adaptive-rho scheme (residual balancing).
<code>tol.abs</code>	A numeric value > 0 (default = 1e-04) specifying the absolute tolerance for ADMM stopping (applied to primal/dual residual norms).
<code>tol.rel</code>	A numeric value > 0 (default = 1e-04) specifying the relative tolerance for ADMM stopping (applied to primal/dual residual norms).
<code>maxiter</code>	An integer (default = 1e+04) specifying the maximum number of ADMM iterations.
<code>crit</code>	A character string (default = "BIC") specifying the parameter selection criterion to use. Available options include: 1. "AIC": Akaike information criterion (Akaike 1973). 2. "BIC": Bayesian information criterion (Schwarz 1978). 3. "EBIC": extended Bayesian information criterion (Chen and Chen 2008; Foygel and Drton 2010). 4. "HBIC": high dimensional Bayesian information criterion (Wang et al. 2013; Fan et al. 2017). 5. "CV": k-fold cross validation with negative log-likelihood loss.
<code>kfold</code>	An integer (default = 5) specifying the number of folds used for <code>crit = "CV"</code> .
<code>ebic.tuning</code>	A numeric value in [0,1] (default = 0.5) specifying the tuning parameter to calculate for <code>crit = "EBIC"</code> .

Value

An object with S3 class "grasps" containing the following components:

hatOmega The estimated precision matrix.

lambda The optimal regularization parameter.

alpha The optimal mixing parameter.

initial The initial estimate of hatOmega when a non-convex penalty is chosen via `penalty`.

- gamma** The optimal additional parameter when a non-convex penalty is chosen via penalty.
- iterations** The number of ADMM iterations.
- lambda.grid** The actual lambda grid used in the program.
- alpha.grid** The actual alpha grid used in the program.
- lambda.safe** The conservative upper bound used to initialize the line search for $\lambda_{\max}$, corresponding to each distinct value in `alpha.grid`, when `lambda = NULL`.
- loss** The optimal k-fold loss when `crit = "CV"`.
- CV.loss** Matrix of CV losses, with rows for parameter combinations and columns for CV folds, when `crit = "CV"`.
- score** The optimal information criterion score when `crit` is set to "AIC", "BIC", "EBIC", or "HBIC".
- IC.score** The information criterion score for each parameter combination when `crit` is set to "AIC", "BIC", "EBIC", or "HBIC".
- membership** The group membership.

References

- Akaike H (1973). "Information Theory and an Extension of the Maximum Likelihood Principle." In Petrov BN, Csáki F (eds.), *Second International Symposium on Information Theory*, 267–281. Akadémiai Kiadó, Budapest, Hungary.
- Candès EJ, Wakin MB, Boyd SP (2008). "Enhancing Sparsity by Reweighted ℓ_1 Minimization." *Journal of Fourier Analysis and Applications*, **14**(5), 877–905. doi:10.1007/s000410089045x.
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- Fan J, Feng Y, Wu Y (2009). "Network Exploration via the Adaptive LASSO and SCAD Penalties." *The Annals of Applied Statistics*, **3**(2), 521–541. doi:10.1214/08aoas215.
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- Fan J, Liu H, Ning Y, Zou H (2017). "High Dimensional Semiparametric Latent Graphical Model for Mixed Data." *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **79**(2), 405–421. doi:10.1111/rssb.12168.
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- Frank LE, Friedman JH (1993). "A Statistical View of Some Chemometrics Regression Tools." *Technometrics*, **35**(2), 109–135. doi:10.1080/00401706.1993.10485033.

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Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
sim <- gen_prec_sbm(p = 30, K = 3,
                   within.prob = 0.25, between.prob = 0.05,
                   weight.dists = list("gamma", "unif"),
                   weight.paras = list(c(shape = 20, rate = 10),
                                       c(min = 0, max = 5)),
                   cond.target = 100)

## ground truth visualization
plot(sim)

## n-by-p data matrix
library(MASS)
X <- mvrnorm(n = 20, mu = rep(0, 30), Sigma = sim$Sigma)

## precision matrix: adaptive lasso; BIC
```

```

prec <- grasps(X = X, membership = sim$membership, penalty = "adapt", crit = "BIC")

## precision matrix visualization
plot(prec)

## performance
performance(hatOmega = prec$hatOmega, Omega = sim$Omega)

## adjacency matrix: diagonal = 0; raw partial correlations;
##                               no thresholding; weighted network
adj <- prec_to_adj(prec$hatOmega,
                  diag.zero = TRUE, absolute = FALSE,
                  threshold = NULL, weighted = TRUE)

## adjacency matrix visualization
plot(adj)

```

performance

Performance Measures for Precision Matrix Estimation

Description

Compute a collection of loss-based and structure-based measures to evaluate the performance of an estimated precision matrix.

Usage

```
performance(hatOmega, Omega)
```

Arguments

hatOmega	A numeric $p \times p$ matrix giving the estimated precision matrix.
Omega	A numeric $p \times p$ matrix giving the reference (typically true) precision matrix.

Details

Let $\Omega_{p \times p}$ and $\hat{\Omega}_{p \times p}$ be the reference (true) and estimated precision matrices, respectively, with $\Sigma = \Omega^{-1}$ being the corresponding covariance matrix. Edges are defined by nonzero off-diagonal entries in the upper triangle of the precision matrices.

Sparsity is treated as a structural summary, while the remaining measures are grouped into loss-based measures, raw confusion-matrix counts, and classification-based (structure-recovery) measures.

"sparsity": Sparsity is computed as the proportion of zero entries among the off-diagonal elements in the upper triangle of $\hat{\Omega}$.

Loss-based measures:

- "Frobenius": Frobenius (Hilbert-Schmidt) norm loss = $\|\Omega - \hat{\Omega}\|_F$.

- "KL": Kullback-Leibler divergence = $\text{tr}(\Sigma\hat{\Omega}) - \log \det(\Sigma\hat{\Omega}) - p$.
- "quadratic": Quadratic norm loss = $\|\Sigma\hat{\Omega} - I_p\|_F^2$.
- "spectral": Spectral (operator) norm loss = $\|\Omega - \hat{\Omega}\|_{2,2} = e_1$, where e_1^2 is the largest eigenvalue of $(\Omega - \hat{\Omega})^2$.

Confusion-matrix counts:

- "TP": True positive = number of edges in both Ω and $\hat{\Omega}$.
- "TN": True negative = number of edges in neither Ω nor $\hat{\Omega}$.
- "FP": False positive = number of edges in $\hat{\Omega}$ but not in Ω .
- "FN": False negative = number of edges in Ω but not in $\hat{\Omega}$.

Classification-based (structure-recovery) measures:

- "TPR": True positive rate (TPR), recall, sensitivity = $\text{TP}/(\text{TP} + \text{FN})$.
- "FPR": False positive rate (FPR) = $\text{FP}/(\text{FP} + \text{TN})$.
- "F1": F_1 score = $2 \text{TP}/(2 \text{TP} + \text{FN} + \text{FP})$
- "MCC": Matthews correlation coefficient (MCC) = $(\text{TP} \times \text{TN} - \text{FP} \times \text{FN}) / \sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}$

The following table summarizes the confusion matrix and related rates:

	Predicted Positive	Predicted Negative
Real Positive (P)	True positive (TP)	False negative (FN)
Real Negative (N)	False positive (FP)	True negative (TN)
	Positive predictive value (PPV), precision = $\text{TP} / (\text{TP} + \text{FP}) = 1 - \text{FDR}$	False omission rate (FOR) = $\text{FN} / (\text{FN} + \text{TN})$
	False discovery rate (FDR) = $\text{FP} / (\text{TP} + \text{FP}) = 1 - \text{PPV}$	Negative predictive value (NPV) = $\text{TN} / (\text{FN} + \text{TN})$

Value

A data frame of S3 class "performance", with one row per performance metric and two columns:

measure The name of each performance metric. The reported metrics include: sparsity, Frobenius norm loss, Kullback-Leibler divergence, quadratic norm loss, spectral norm loss, true positive, true negative, false positive, false negative, true positive rate, false positive rate, F1 score, and Matthews correlation coefficient.

value The corresponding numeric value.

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
sim <- gen_prec_sbm(p = 30, K = 3,
  within.prob = 0.25, between.prob = 0.05,
  weight.dists = list("gamma", "unif"),
```

```

weight.paras = list(c(shape = 20, rate = 10),
                    c(min = 0, max = 5)),
cond.target = 100)

## ground truth visualization
plot(sim)

## n-by-p data matrix
library(MASS)
X <- mvrnorm(n = 20, mu = rep(0, 30), Sigma = sim$Sigma)

## precision matrix: adaptive lasso; BIC
prec <- grasps(X = X, membership = sim$membership, penalty = "adapt", crit = "BIC")

## precision matrix visualization
plot(prec)

## performance
performance(hatOmega = prec$hatOmega, Omega = sim$Omega)

## adjacency matrix: diagonal = 0; raw partial correlations;
## no thresholding; weighted network
adj <- prec_to_adj(prec$hatOmega,
                  diag.zero = TRUE, absolute = FALSE,
                  threshold = NULL, weighted = TRUE)

## adjacency matrix visualization
plot(adj)

```

plot.adjmat

*Plot Function for S3 Class "adjmat"***Description**

Visualize an adjacency matrix as a heatmap. This function is shared by objects returned from [prec_to_adj](#).

Usage

```
## S3 method for class 'adjmat'
plot(x, ...)
```

Arguments

x An object inheriting from S3 class "adjmat", typically returned by [prec_to_adj](#).
... Additional arguments passed to [ggplot](#).

Value

A heatmap of class `ggplot` showing the matrix entries. The plot title also reports matrix dimension and sparsity.

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
sim <- gen_prec_sbm(p = 30, K = 3,
  within.prob = 0.25, between.prob = 0.05,
  weight.dists = list("gamma", "unif"),
  weight.paras = list(c(shape = 20, rate = 10),
    c(min = 0, max = 5)),
  cond.target = 100)

## ground truth visualization
plot(sim)

## n-by-p data matrix
library(MASS)
X <- mvrnorm(n = 20, mu = rep(0, 30), Sigma = sim$Sigma)

## precision matrix: adaptive lasso; BIC
prec <- grasps(X = X, membership = sim$membership, penalty = "adapt", crit = "BIC")

## precision matrix visualization
plot(prec)

## performance
performance(hatOmega = prec$hatOmega, Omega = sim$Omega)

## adjacency matrix: diagonal = 0; raw partial correlations;
## no thresholding; weighted network
adj <- prec_to_adj(prec$hatOmega,
  diag.zero = TRUE, absolute = FALSE,
  threshold = NULL, weighted = TRUE)

## adjacency matrix visualization
plot(adj)
```

plot.blkmat

Plot Function for Block-Structured Precision Matrices (Visualize a Matrix with Group Boundaries)

Description

Visualize a precision matrix as a heatmap with dashed boundary lines separating group blocks. This function is shared by objects returned from [grasps](#), [gen_prec_sbm](#), and [sparsify_block_banded](#), all of which inherit from the S3 class "blkmat".

Usage

```
## S3 method for class 'blkmat'
plot(x, colors = NULL, ...)
```

Arguments

x An object inheriting from S3 class "blkmat", typically returned by [grasps](#), [gen_prec_sbm](#) or [sparsify_block_banded](#).

colors A vector of colors specifying an n-color gradient scale for the fill aesthetics.

... Additional arguments passed to [ggplot](#).

Value

A heatmap of class ggplot showing the matrix entries. Dashed lines indicate group boundaries. The plot title also reports matrix dimension and sparsity.

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
sim <- gen_prec_sbm(p = 100, K = 10,
  within.prob = 0.2, between.prob = 0.05,
  weight.dists = list("gamma", "unif"),
  weight.paras = list(c(shape = 100, scale = 10),
    c(min = 0, max = 5)),
  cond.target = 100)

## visualization
plot(sim)
```

plot.penderiv

Plot Function for S3 Class "penderiv"

Description

Generate a visualization of penalty functions produced by [compute_penalty](#), or penalty derivatives produced by [compute_derivative](#). The plot automatically summarizes multiple configurations of penalty type, λ , and γ . Optional zooming is supported through [facet_zoom](#).

Usage

```
## S3 method for class 'penderiv'
plot(x, ...)
```

Arguments

- x An object inheriting from S3 class "penderiv", typically returned by `compute_penalty`, or `compute_derivative`.
- ... Optional arguments passed to `facet_zoom` to zoom in on a subset of the data, while keeping the view of the full dataset as a separate panel.

Value

An object of class `ggplot`.

Examples

```
library(grasps)
library(ggplot2)

pen_df <- compute_penalty(
  omega = seq(-4, 4, by = 0.01),
  penalty = c("atan", "exp", "lasso", "lq", "lsp", "mcp", "scad"),
  lambda = 1)

plot(pen_df, xlim = c(-1, 1), ylim = c(0, 1), zoom.size = 1) +
  guides(color = guide_legend(nrow = 2, byrow = TRUE))

deriv_df <- compute_derivative(
  omega = seq(0, 4, by = 0.01),
  penalty = c("atan", "exp", "lasso", "lq", "lsp", "mcp", "scad"),
  lambda = 1)

plot(deriv_df) +
  scale_y_continuous(limits = c(0, 1.5)) +
  guides(color = guide_legend(nrow = 2, byrow = TRUE))
```

```
prec_to_adj
```

Adjacency Matrix from Precision Matrix

Description

Convert a precision matrix to a partial-correlation-based adjacency matrix.

Usage

```
prec_to_adj(
  prec.mat,
  diag.zero = TRUE,
  absolute = FALSE,
  threshold = NULL,
  weighted = TRUE
)
```

Arguments

prec.mat	A numeric precision matrix.
diag.zero	A logical value (default = TRUE) specifying whether to set the diagonal entries of the adjacency matrix to 0. If diag.zero = FALSE, the diagonal entries are set to 1 for a weighted network. For an unweighted network (weighted = FALSE), the diagonal is always forced to 0 to avoid self-loops.
absolute	A logical value (default = FALSE) specifying whether to take the absolute values of the partial correlations.
threshold	A nonnegative numeric value (default = NULL) specifying the threshold for edge filtering. Entries with absolute values smaller than the threshold are set to 0.
weighted	A logical value (default = TRUE) specifying whether to return a weighted adjacency matrix. If weighted = FALSE, the matrix is a binary adjacency matrix with entries equal to 0 or 1.

Details

For a precision matrix Ω , the partial correlation between nodes i and j is computed as

$$\rho_{ij} = -\frac{\Omega_{ij}}{\sqrt{\Omega_{ii}\Omega_{jj}}}.$$

Value

A numeric adjacency matrix with S3 class "adjmat".

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## block-structured precision matrix based on SBM
sim <- gen_prec_sbm(p = 30, K = 3,
  within.prob = 0.25, between.prob = 0.05,
  weight.dists = list("gamma", "unif"),
  weight.paras = list(c(shape = 20, rate = 10),
    c(min = 0, max = 5)),
  cond.target = 100)

## ground truth visualization
plot(sim)

## n-by-p data matrix
library(MASS)
X <- mvrnorm(n = 20, mu = rep(0, 30), Sigma = sim$Sigma)

## precision matrix: adaptive lasso; BIC
prec <- grasps(X = X, membership = sim$membership, penalty = "adapt", crit = "BIC")

## precision matrix visualization
```

```

plot(prec)

## performance
performance(hatOmega = prec$hatOmega, Omega = sim$Omega)

## adjacency matrix: diagonal = 0; raw partial correlations;
##                      no thresholding; weighted network
adj <- prec_to_adj(prec$hatOmega,
                  diag.zero = TRUE, absolute = FALSE,
                  threshold = NULL, weighted = TRUE)

## adjacency matrix visualization
plot(adj)

```

sparsify_block_banded *Groupwise Block-Banded Sparsifier*

Description

Make a precision-like matrix block-banded according to group membership, keeping only entries within specified group neighborhoods.

Usage

```
sparsify_block_banded(mat, membership, neighbor.range = 1)
```

Arguments

<code>mat</code>	A $p \times p$ precision-like matrix specifying the base matrix to be masked.
<code>membership</code>	An integer vector specifying the group membership. The length of membership must be consistent with the dimension p .
<code>neighbor.range</code>	An integer (default = 1) specifying the neighbor range, where groups whose labels differ by at most <code>neighbor.range</code> are considered neighbors and kept in the mask.

Value

An object with S3 class "sparsify_block_banded" containing the following components:

Omega The masked precision matrix.

Sigma The covariance matrix, i.e., the inverse of Omega.

sparsity Proportion of zero entries in Omega.

membership An integer vector specifying the group membership.

Examples

```
library(grasps)

## reproducibility for everything
set.seed(1234)

## precision matrix estimation
X <- matrix(rnorm(200), 10, 20)
membership <- c(rep(1,5), rep(2,5), rep(3,4), rep(4,6))
est <- grasps(X, membership = membership, penalty = "lasso", crit = "BIC")

## default: keep blocks within  $\pm 1$  of each group
res1 <- sparsify_block_banded(est$hatOmega, membership, neighbor.range = 1)
plot(res1)

## wider band: keep blocks within  $\pm 2$  of each group
res2 <- sparsify_block_banded(est$hatOmega, membership, neighbor.range = 2)
plot(res2)

## special case: block-diagonal matrix
res3 <- sparsify_block_banded(est$hatOmega, membership, neighbor.range = 0)
plot(res3)
```

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