Package ‘sparseHessianFD’

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Type Package

Title Numerical Estimation of Sparse Hessians

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Maintainer Michael Braun <braunm@smu.edu>

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Description Estimates Hessian of a scalar-valued function, and returns it in a sparse Matrix format. The sparsity pattern must be known in advance. The algorithm is especially efficient for hierarchical models with a large number of heterogeneous units.

License MPL (== 2.0)

LazyData true

Depends R (>= 3.2.3)

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Suggests testthat, numDeriv, scales, knitr, xtable, dplyr

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Author Michael Braun [aut, cre, cph]

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R topics documented:

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sparseHessianFD-package

Estimate sparse Hessians using finite differences of gradients.

Description

Estimate sparse Hessians using finite differences of gradients.

Details

The Hessian is returned as a sparse Matrix (dgCMatrix-class). The user supplies the objective function, the gradient, and the row and column indices of the non-zero elements of the lower triangle of the Hessian (i.e., the sparsity structure must be known in advance).

In a typical case, you should only need to use the sparseHessianFD initializer, and the fn, gr and hessian methods of the sparseHessian class, and the Matrix.to.Coord utility function.

References


**Description**

Functions for binary choice example in the vignette.

**Usage**

\[
\begin{align*}
\text{binary.f}(P, \text{data}, \text{priors}, \text{order.row} = \text{FALSE}) \\
\text{binary.grad}(P, \text{data}, \text{priors}, \text{order.row} = \text{FALSE}) \\
\text{binary.hess}(P, \text{data}, \text{priors}, \text{order.row} = \text{FALSE})
\end{align*}
\]

**Arguments**

- **P**: Numeric vector of length \((N + 1)k\). First \(Nk\) elements are heterogeneous coefficients. The remaining \(k\) elements are population parameters.
- **data**: Named list of data matrices \(Y\) and \(X\), and choice count integer \(T\)
- **priors**: Named list of matrices \(\text{inv.Omega}\) and \(\text{inv.Sigma}\)
- **order.row**: Determines order of heterogeneous coefficients in parameter vector. If TRUE, heterogeneous coefficients are ordered by unit. If FALSE, they are ordered by covariate.

**Details**

These functions are used by the heterogeneous binary choice example in the vignette. There are \(N\) heterogeneous units, each making \(T\) binary choices. The choice probabilities depend on \(k\) covariates.

**Value**

Log posterior density, gradient and Hessian. The Hessian is a dgCMatrix object.

---

**binary-data**

*Sample simulated data for binary choice example in vignette*

**Description**

Sample datasets for vignette
Details

The package provides four sample datasets for the hierarchical binary choice model described in the vignette. These datasets are:

- **binary** \( N = 50, k = 3 \)
- **binary_small** \( N = 20, k = 2 \)
- **binary_large** \( N = 800, k = 3 \)
- **binary_super** \( N = 1200, k = 3 \)

\( N \) is the number of heterogeneous units. \( k \) is the number of covariates.

The datasets were generated using the code in `data-raw/binary_sim.R`.

---

**coloring**

*Triangular partitioning of variables*

---

Description

Cyclic coloring from a lower triangular pattern matrix

Usage

```r
coloring(L)
```

Arguments

- `L` 
  sparsity pattern of the Hessian as a lower triangular pattern matrix

Details

For internal use. Exported in order for replication files for JSS article to run.

Value

Integer vector of length `nvars` with color assignments for each variable.
Coord.to.Pointers

Convert a matrix defined by row and column indices to one defined by a row- or column-oriented compression scheme.

Description

Returns indices and pointers that define a sparse Hessian in compressed format. Inputs are the row and column indices.

Usage

Coord.to.Pointers(rows, cols, dims, triangle = TRUE, lower = TRUE, symmetric = FALSE, order = c("column", "row", "triplet"), index1 = TRUE)

Arguments

rows, cols row and column indices of non-zero elements
dims 2-element vector for number of rows and columns.
triangle Is input intended to be a triangular (TRUE) or full (FALSE) matrix. See details for how this argument is interpreted for different values of order.
lower If triangular is true, this argument identifies the input matrix as lower- or upper-triangular. This argument is ignored if triangle is FALSE.
symmetric If TRUE, and matrix is triangular, then the matrix will be treated as symmetric, with only the triangular elements provided. If matrix is neither triangular nor symmetric, then symmetric=TRUE will probably trigger an error.
order Determines the indexing/compression scheme for the output matrix. Use "triplet" to get row and column indices. Defaults to the same class as M.
index1 TRUE if using 1-based indexing. FALSE for 0-based indexing.

Details

triangle and order have the following interpretation:

triangle=TRUE Input rows and cols represent lower or upper triangle of a matrix. If order="symmetric", then the output list will be for a full, symmetric matrix. Otherwise, the output list will be for only the lower or upper triangle. Any elements outside of the specified triangle will trigger an error.

triangle=FALSE Input rows and cols represent a full matrix. If that matrix is not symmetric, then order="symmetric" will trigger an error. If symmetric=FALSE and order='triplet', the output list should contain the same row and column indices as the input list.

Value

A list. See Matrix.to.Pointers (no values are included in return list).
See Also

Matrix.to.Pointers

deprecated

**Deprecated functions**

**Description**

These functions were in earlier versions, but will no longer be maintained, and are not even guaranteed to work now.

Build sparse matrix from data in CSC (column compressed) format.

Converts row and column indices to a pattern Matrix object of Matrix class.

This function is deprecated. Use `sparseHessianFD` instead.

**Usage**

Sym.CSC.to.Matrix(H, nvars)

Coord.to.Sym.Pattern.Matrix(H, nvars)

Coord.to.Pattern.Matrix(rows, cols, dims, compressed = TRUE,
  symmetric = FALSE, index1 = TRUE)

new.sparse.hessian.obj(x, fn, gr, hs, fd.method = 0L,
  eps = sqrt(.Machine$double.eps), ...)

sparseHessianFD.new(x, fn, gr, rows, cols, direct = NULL,
  eps = sqrt(.Machine$double.eps), ...)

**Arguments**

- **H**: a list containing Hessian data. See details.
- **nvars**: the number of rows (and columns) in the matrix.
- **rows, cols**: row and column indices of non-zero elements
- **dims**: 2-element vector for number of rows and columns in matrix
- **compressed**: If TRUE, returns a matrix is compressed column (default=TRUE)
- **symmetric**: If TRUE, matrix will be symmetric, and only the lower triangular elements need to be provided (default=FALSE)
- **index1**: TRUE if input row and col use 1-based indexing, and FALSE for 0-based indexing.
- **x**: variable vector for initialization
- **fn**: R function that returns function value
- **gr**: R function that returns the gradient of the function
get_colors

hs list of two vectors: row and column indices of non-zero elements of lower triangle of Hessian. See details.

fd.method If TRUE, use direct method for computation. Otherwise, use indirect/substitution method. See references.

eps The perturbation amount for finite differencing of the gradient to compute the Hessian. Defaults to \text{sqrt(.Machine$double.eps)}.  

... Other parameters to be passed to fn and gr.

direct If TRUE, use direct method for computation. Otherwise, use indirect/substitution method. See references.

Details

Use Matrix::\text{sparseMatrix} instead of Sym.CSC.to.Matrix.
This function is useful to prototype a sparsity pattern. No assumptions are made about symmetry.

hs is a list of two elements:

iRow Integer vector of row indices of non-zero elements in lower triangle of Hessian.

jCol Integer vector of column indices of non-zero elements in lower triangle of Hessian.

This function is deprecated. Use \text{sparseHessianFD} instead.

Value

An object of Matrix class.
A sparse pattern matrix
An object of class \text{sparseHessianFD}

get_colors Vertex coloring of a sparse undirected graph

Description

Generate proper vertex coloring of a sparse undirected graph.

Usage

get_colors(pntr, idx, nvars)

Arguments

pntr, idx row pointers and column indices of the adjacency matrix, in compressed column-oriented format. Must use zero-based indexing.

nvars Number of vertices.
Matrix.to.Coord

Details
For internal use. You should not have to call this function directly.

Value
An integer vector of length nvars, where each element represents the color of the corresponding vertex. Indices are zero-based.

Description
Utility function to extract row and column indices of the non-zero elements of a sparse matrix.

Usage
Matrix.to.Coord(M, index1 = TRUE)

Arguments
M A matrix that is a subclass of sparseMatrix, as defined in the Matrix package.
index1 TRUE if the index of the first element should be 1, and FALSE if 0.

Details
A wrapper to Matrix.to.Pointers for order=‘triplet’ and values=FALSE, for extracting the row and column indices of a sparsity pattern from a matrix that has that same pattern.

Value
A list with two named elements.

rows Integer vector containing row indices of non-zero elements

cols Integer vector containing column indices of non-zero elements

Examples
M1 <- as(kronecker(diag(3), matrix(TRUE,2,2)),”sparseMatrix”)
C <- Matrix.to.Coord(M1)
M2 <- Matrix::sparseMatrix(i=C$rows, j=C$cols)
all.equal(M1,M2)
Matrix.to.Pointers

Extract row and column indices, pointers and values from a sparse matrix.

Description

Returns a list of row indices, column indices, pointers, and/or values of a sparse Hessian.

Usage

Matrix.to.Pointers(M, as.symmetric = Matrix::isSymmetric(M), values = !is(M, "nMatrix"), order = NULL, index1 = TRUE)

Arguments

- **M**: A sparse Matrix, as defined in the Matrix package.
- **as.symmetric**: Defaults to isSymmetric(M). If M is symmetric, and as.symmetric is FALSE, then index/pointer elements in the output list will be labeled according to order. If M is not symmetric, and as.symmetric is TRUE, then an error will be triggered.
- **values**: If TRUE, values are returned in list as 'x'. Defaults to TRUE for numeric and logical matrices, and FALSE for pattern matrices. If M is a pattern matrix, values=TRUE will trigger a warning.
- **order**: Determines the indexing/compression scheme for the output matrix. Use 'triplet' to get row and column indices. Defaults to the same class as M.
- **index1**: TRUE (default) if return indices and pointers should use 1-based indexing. FALSE for 0-based indexing.

Details

This function is included primarily for debugging purposes. It is used internally, but would not ordinarily be called by an end user.

Value

A list with the following elements. If order=='row',

- **jCol**: Integer vector containing column indices of non-zero elements
- **ipntr**: Integer vector containing pointers to elements of jCol at which the next row begins.

If order=='column'

- **iRow**: Integer vector containing row indices of non-zero elements
- **jpntr**: Integer vector containing pointers to elements of iRow at which the next column begins.

If order=='triplet'

- **rows**: Row indices of non-zero elements
A reference class for computing sparse Hessians

The `sparseHessianFD` function calls the initializer for the `sparseHessianFD` class, and returns a `sparseHessianFD` object.

```r
sparseHessianFD(x, fn, gr, rows, cols, delta, index1, complex, ...)
```

The function, gradient and sparsity pattern are declared as part of the initialization. Once initialized, the `$hessian` method will evaluate the Hessian at x.

```r
obj <- sparseHessian(x, fn, gr, rows, cols, ...)
obj$hessian(x)
```

For convenience, the class provides wrapper methods to the `fn` and `gr` functions that were specified in the initializer.

```r
obj$fn(P) ## wrapper to objective function
obj$gr(P) ## wrapper to gradient
obj$fngr(P) ## list of obj function and gradient
obj$fngrhs(P) ## list of obj function, gradient and Hessian.
```

**Arguments to initializer:**
- `x` an vector at which the function, gradient and Hessian are initialized and tested.
- `fn, gr` R functions that return the function value and gradient, evaluated at x.
- `rows, cols` Numeric vectors with row and column indices of the non-zero elements in the lower triangle (including diagonal) of the Hessian.

**Description**

A reference class for computing sparse Hessians

**Details**

The `sparseHessianFD` function calls the initializer for the `sparseHessianFD` class, and returns a `sparseHessianFD` object.
**delta**  The perturbation amount for finite difference (or complex step) of the gradient to compute the Hessian. Defaults to 1e-07.

**index1**  TRUE if rows and cols use 1-based (R format) indexing (FALSE for 0-based (C format) indexing.

**complex**  TRUE if Hessian will be computed using the complex step method, and FALSE (default) if using finite differences. If TRUE, both fn and gr must accept complex arguments and return complex values.

... other arguments to be passed to fn and gr.

Other methods are described below. Do not access any of the fields directly. The internal structure is subject to change in future versions.

**Fields**

- **fn1**  A closure for calling fn(x, ...).
- **gr1**  A closure for calling gr(x, ...).
- **iRow, jCol**  Numeric vectors with row and column indices of the non-zero elements in the lower triangle (including diagonal) of the Hessian.
- **delta**  The perturbation amount for finite differencing of the gradient to compute the Hessian. Defaults to 1e-07.
- **index1**  TRUE if rows and cols use 1-based (R format) indexing (FALSE for 0-based (C format) indexing.
- **complex**  TRUE if Hessian will be computed using the complex step method, and FALSE (default) if using finite differences.
- **D**  raw finite differences (internal use only)
- **nvars**  Number of variables (length of x)
- **nnz**  Number of non-zero elements in the lower triangle of the Hessian.
- **ready**  TRUE if object has been initialized, and Hessian has been partitioned.
- **idx, pnttr**  Column indices and row pointers for non-zero elements in lower triangle of the permuted Hessian. Row-oriented compressed storage.
- **colors**  A vector representation of the partitioning of the columns. There are nvars elements, one for each column of the permuted Hessian. The value corresponds to the "color" for that column.
- **perm, invperm**  Permutation vector and its inverse

**Methods**

- **fn(x)**  Return function value, evaluated at x: fn(x, ...)
- **fngr(x)**  Return list of function value and gradient, evaluated at x
- **fngrhs(x)**  Return list of function value, gradient, and Hessian, evaluated at x
- **get_invperm()**  Return integer vector of inverse of permutation used for computing Hessian
- **get_nnz()**  Return number of non-zero elements in lower triangle of Hessian
- **get_nvars()**  Return dimension (number of rows or columns) of Hessian
get_pattern() Return pattern matrix of lower triangle of Hessian
get_perm() Return integer vector of permutation used for computing Hessian
get_perm_pattern() Return pattern matrix of lower triangle of *permuted* Hessian
g(x) Return gradient, evaluated at x: gr(x,...)
hessian(x) Return sparse Hessian, evaluated at x, as a dgCMatrix object.
initialize(x, fn, gr, rows, cols, delta = 1e-07, index1 = TRUE, complex = FALSE, ...)
    Initialize object with functions to compute the objective function and gradient (fn and gr), row
    and column indices of non-zero elements (rows and cols), an initial variable vector x at which
    fn and gr can be evaluated, a finite differencing parameter delta, flags for 0 or 1-based index-
    ing (index1), whether the complex step method will be used, and other arguments (...) to be
    passed to fn and gr.
partition() Return the partitioning used to compute finite differences
pointers(out,index1 = index1) Return list with indices (idx) and pointers (pntr) for sparsity
    pattern of the compressed sparse Hessian. Since the Hessian is symmetric, the indices and
    pointers for row-oriented and column-oriented storage patterns are the same.

Examples

```r
## Log posterior density of hierarchical binary choice model. See vignette.
set.seed(123)
data("binary_small")
N <- length(binary["Y"])
k <- NROW(binary["X"])
T <- binary["T"]
P <- rnorm((N+1)*k)
priors <- list(inv.Sigma = rWishart(1,k+5,diag(k))[,1],
               inv.Omega = diag(k))
true.hess <- binary.hess(P, binary, priors)
pattern <- Matrix.to.Coord(Matrix::tril(true.hess))
str(pattern)
obj <- sparseHessianFD(P, fn=binary.f, gr=binary.grad, rows=pattern["rows"], cols=pattern["cols"],
                        data=binary, priors=priors)
hs <- obj$hessian(P)
all.equal(hs, true.hess)

f <- obj$fn(P) ## obj function
df <- obj$gr(P) ## gradient
fdf <- obj$fngP) ## list of obj function and gradient
fdfhs <- obj$fngrhs(P) ## list of obj function, gradient and Hessian.
```

### Estimate sparse Hessian

**Description**

Estimate Hessian using triangular substitution algorithm
Usage

\texttt{subst(Y, colors, jCol, ipntr, delta, nvars, nnz)}

Arguments

\begin{itemize}
  \item \texttt{Y} \hspace{1cm} \text{Matrix of finite differences of gradients}
  \item \texttt{colors} \hspace{1cm} \text{Vector of length nvars that identifies color of each variable}
  \item \texttt{jCol, ipntr} \hspace{1cm} \text{Column indices and row pointers for non-zero elements of lower triangle of Hessian (row-oriented compressed format).}
  \item \texttt{delta} \hspace{1cm} \text{Perturbation factor used to compute finite differences of gradients.}
  \item \texttt{nvars} \hspace{1cm} \text{Dimension of Hessian (number of variables)}
  \item \texttt{nnz} \hspace{1cm} \text{Number of non-zero elements in the lower triangle of the Hessian.}
\end{itemize}

Details

For internal use. You should not have to call this function directly.

Value

A sparse Hessian of class \texttt{dgCMatrix}.\"
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