Package 'fntl'

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Title Numerical Tools for 'Rcpp' and Lambda Functions

Version 0.1.1

Description Provides a 'C++' API for routinely used numerical tools such as integration, root-finding, and optimization, where function arguments are given as lambdas. This facilitates 'Rcpp' programming, enabling the development of 'R'-like code in 'C++' where functions can be defined on the fly and use variables in the surrounding environment.

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URL https://github.com/andrewraim/fntl

Depends R (>= 4.3)

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Imports Rcpp

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NeedsCompilation yes

Author Andrew M. Raim [aut, cre] (<https://orcid.org/0000-0002-4440-2330>)

Maintainer Andrew M. Raim <andrew.raim@gmail.com>

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Package documentation

Author(s)

Maintainer: Andrew M. Raim <andrew.raim@gmail.com> (ORCID)

See Also

Useful links:

- https://github.com/andrewraim/fntl

`args` *Arguments*

Description

Get an arguments list for internal methods with the default settings. This object can be adjusted and passed to the respective function.

Usage

```
findroot_args()

optimize_args()

integrate_args()

cg_args()

bfgs_args()
```

```
lbfgsb_args()

neldermead_args()

nlm_args()

richardson_args()
```

Value

An argument list corresponding to the specified function. The elements of the list are named and supplied with default values. See the package vignette for further details.

- `findroot_args` is documented in the section "Root-Finding".
- `optimize_args` is documented in the section "Univariate Optimization".
- `integrate_args` is documented in the section "Integration".
- `cg_args` is documented in the section "Conjugate Gradient".
- `bfgs_args` is documented in the section "BFGS".
- `lbfgsb_args` is documented in the section "L-BFGS-B".
- `neldermead_args`is documented in the section "Nelder-Mead".
- `nlm_args` is documented in the section "Newton-Type Algorithm for Nonlinear Optimization".
- `richardson_args` is documented in the section "Richardson Extrapolated Finite Differences".

`deriv` *Numerical Derivatives via Finite Differences*

Description

Numerical Derivatives via Finite Differences

Usage

```
fd_deriv1(f, x, i, h, fd_type)

fd_deriv2(f, x, i, j, h_i, h_j, fd_type)

deriv1(f, x, i, args, fd_type)

deriv2(f, x, i, j, args, fd_type)
```

Arguments

f	Function to differentiate.
x	Scalar at which to evaluate the derivative.
i	First coordinate to differentiate.
h	Step size in the first coordinate.
fd_type	Type of derivative: 0 for symmetric difference, 1 for forward difference, and 2 for backward difference.
j	Second coordinate to differentiate.
h_i	Step size in the first coordinate.
h_j	Step size in the second coordinate.
args	List of additional arguments from the function richardson_args.

Value

fd_deriv1 and fd_deriv2 return a single numeric value corresponding to the first and second derivative via finite differences. deriv1 and deriv2 return a list with the form of a richardson_result described in section "Richardson Extrapolated Finite Differences" of the package vignette.

Examples

```
args = richardson_args()

f = sin   # Try 2nd derivatives of a univariate function
x0 = 0.5
print(-sin(x0))  ## Exact answer for f''(x0)

fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 0)
fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 1)
fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 2)

deriv2(f, x0, i = 0, j = 0, args, fd_type = 0)

# Try 2nd derivatives of a bivariate function
f = function(x) { sin(x[1]) + cos(x[2]) }
x0 = c(0.5, 0.25)

print(-sin(x0[1]))  ## Exact answer for f_xx(x0)
print(-cos(x0[2]))  ## Exact answer for f_yy(x0)
print(0)         ## Exact answer for f_xy(x0,y0)

numDeriv::hessian(f, x0)

fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 0)
fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 1)
fd_deriv2(f, x0, i = 0, j = 0, h_i = 0.001, h_j = 0.001, fd_type = 2)

fd_deriv2(f, x0, i = 0, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 0)
fd_deriv2(f, x0, i = 0, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 1)
```

```
fd_deriv2(f, x0, i = 0, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 2)

fd_deriv2(f, x0, i = 1, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 0)
fd_deriv2(f, x0, i = 1, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 1)
fd_deriv2(f, x0, i = 1, j = 1, h_i = 0.001, h_j = 0.001, fd_type = 2)

deriv2(f, x0, i = 1, j = 1, args, fd_type = 0)
deriv2(f, x0, i = 1, j = 1, args, fd_type = 1)
deriv2(f, x0, i = 1, j = 1, args, fd_type = 2)
```

`findroot` *Find Root*

Description

Find Root

Usage

```
findroot_bisect(f, lower, upper, args)

findroot_brent(f, lower, upper, args)
```

Arguments

`f`	Function for which a root is desired.
`lower`	Lower limit of search interval. Must be finite.
`upper`	Upper limit of search interval. Must be finite.
`args`	List of additional arguments from the function `findroot_args`.

Value

A list with the form of a `findroot_result` described in section "Root-Finding" of the package vignette.

Examples

```
f = function(x) { x^2 - 1 }
args = findroot_args()
findroot_bisect(f, 0, 10, args)
findroot_brent(f, 0, 10, args)
```

gradient0 *Numerical Gradient Vector*

Description

Numerical Gradient Vector

Usage

```
gradient0(f, x, args)
```

Arguments

f	Function to differentiate.
x	Vector at which to evaluate the gradient.
args	List of additional arguments from the function `richardson_args`.

Value

A list with the form of a `gradient_result` described in section "Gradient" of the package vignette.

Examples

```
f = function(x) { sum(sin(x)) }
args = richardson_args()
x0 = seq(0, 1, length.out = 5)
cos(x0)  ## Exact answer
gradient0(f, x0, args)
numDeriv::grad(f, x0)
```

hessian0 *Numerical Hessian*

Description

Numerical Hessian

Usage

```
hessian0(f, x, args)
```

Arguments

f	Function to differentiate.
x	Vector at which to evaluate the Hessian.
args	List of additional arguments from the function `richardson_args`.

Value

A list with the form of a `hessian_result` described in section "Hessian" of the package vignette.

Examples

```
f = function(x) { sum(x^2) }
x0 = seq(1, 10, length.out = 5)
args = richardson_args()
hessian0(f, x0, args)
numDeriv::hessian(f, x0)
```

`integrate0` *Integration*

Description

Compute the integral $\int_a^b f(x) dx$.

Usage

```
integrate0(f, lower, upper, args)
```

Arguments

`f`	Function to integrate.
`lower`	Lower limit of integral.
`upper`	Upper limit of integral.
`args`	List of additional arguments from the function `integrate_args`.

Value

A list with the form of a `integrate_result` described in section "Integration" of the package vignette.

Examples

```
f = function(x) { exp(-x^2 / 2) }
args = integrate_args()
integrate0(f, 0, 10, args)
```

jacobian0 *Numerical Jacobian Matrix*

Description

Numerical Jacobian Matrix

Usage

```
jacobian0(f, x, args)
```

Arguments

f	Function to differentiate.
x	Vector at which to evaluate the Jacobian.
args	List of additional arguments from the function richardson_args.

Value

A list with the form of a jacobian_result described in section "Jacobian" of the package vignette.

Examples

```
f = function(x) { cumsum(sin(x)) }
x0 = seq(1, 10, length.out = 5)
args = richardson_args()
out = jacobian0(f, x0, args)
print(out$value)
numDeriv::jacobian(f, x0)
```

matrix_apply *Matrix Apply Functions*

Description

Matrix Apply Functions

Usage

```
mat_apply(X, f)

row_apply(X, f)

col_apply(X, f)
```

Arguments

`X`	A matrix
`f`	The function to apply.

Details

The `mat_apply`, `row_apply`, and `col_apply` C++ functions are intended to operate like the following calls in R, respectively.

```
apply(x, c(1,2), f)
apply(x, 1, f)
apply(x, 2, f)
```

The R functions exposed here are specific to numeric-valued matrices, but the underlying C++ functions are intended to work with any type of Rcpp Matrix.

Value

`mat_apply` returns a matrix. `row_apply` and `col_apply` return a vector. See section "Apply" of the package vignette for details.

Examples

```
X = matrix(1:12, nrow = 4, ncol = 3)
mat_apply(X, f = function(x) { x^(1/3) })
row_apply(X, f = function(x) { sum(x^2) })
col_apply(X, f = function(x) { sum(x^2) })
```

---

multivariate-optimization

Multivariate Optimization

Description

Multivariate Optimization

Usage

```
cg1(init, f, g, args)

cg2(init, f, args)

bfgs1(init, f, g, args)

bfgs2(init, f, args)
```

```
lbfgsb1(init, f, g, args)

lbfgsb2(init, f, args)

neldermead(init, f, args)

nlm1(init, f, g, h, args)

nlm2(init, f, g, args)

nlm3(init, f, args)
```

Arguments

init	Initial value
f	Function f to optimize
g	Gradient function of f.
args	List of additional arguments for optimization.
h	Hessian function of f.

Details

The argument args should be a list constructed from one of the following functions:

- bfgs_args for BFGS;
- lbfgsb_args for L-BFGS-B;
- cg_args for CG;
- neldermead_args for Nelder-Mead;
- nlm_args for the Newton-type algorithm used in nlm.

When g or h are omitted, the gradient or Hessian will be respectively be computed via finite differences.

Value

A list with results corresponding to the specified function. See the package vignette for further details.

- cg1 and cg2 return a cg_result which is documented in the section "Conjugate Gradient".
- bfgs1 and bfgs2 return a bfgs_result which is documented in the section "BFGS".
- lbfgsb1 and lbfgsb2 return a lbfgsb_result which is documented in the section "L-BFGS-B".
- neldermead returns a neldermead_result which is documented in the section "Nelder-Mead".
- nlm1, nlm2, and nlm3 return a nlm_result which is documented in the section "Newton-Type Algorithm for Nonlinear Optimization".

Examples

```
f = function(x) { sum(x^2) }
g = function(x) { 2*x }
h = function(x) { 2*diag(length(x)) }
x0 = c(1,1)

args = cg_args()
cg1(x0, f, g, args)
cg2(x0, f, args)

args = bfgs_args()
bfgs1(x0, f, g, args)
bfgs2(x0, f, args)

args = lbfgsb_args()
lbfgsb1(x0, f, g, args)
lbfgsb2(x0, f, args)

args = neldermead_args()
neldermead(x0, f, args)

args = nlm_args()
nlm1(x0, f, g, h, args)
nlm2(x0, f, g, args)
nlm3(x0, f, args)
```

`outer` *Outer Matrix*

Description

Compute "outer" matrices and matrix-vector products based on a function that operators on pairs of rows. See details.

Usage

```
outer1(X, f)

outer2(X, Y, f)

outer1_matvec(X, f, a)

outer2_matvec(X, Y, f, a)
```

Arguments

`X`	A numerical matrix.

f	Function $f(x, y)$ that operates on a pair of rows. Depending on the context, rows x and y are both rows of X, or x is a row from X and y is a row from from Y.
Y	A numerical matrix.
a	A scalar vector.

Details

The `outer1` function computes the $n \times n$ symmetric matrix

$$\text{outer1}(X, f) = \begin{bmatrix} f(x_1, x_1) & \cdots & f(x_1, x_n) \\ \vdots & \ddots & \vdots \\ f(x_n, x_1) & \cdots & f(x_n, x_n) \end{bmatrix}$$

and the `outer1_matvec` operation computes the n-dimensional vector

$$\text{outer1\_matvec}(X, f, a) = \begin{bmatrix} f(x_1, x_1) & \cdots & f(x_1, x_n) \\ \vdots & \ddots & \vdots \\ f(x_n, x_1) & \cdots & f(x_n, x_n) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}.$$

The `outer2` operation computes the $m \times n$ matrix

$$\text{outer2}(X, Y, f) = \begin{bmatrix} f(x_1, y_1) & \cdots & f(x_1, y_n) \\ \vdots & \ddots & \vdots \\ f(x_m, y_1) & \cdots & f(x_m, y_n) \end{bmatrix}$$

and the `outer2_matvec` operation computes the m-dimensional vector

$$\text{outer2\_matvec}(X, Y, f, a) = \begin{bmatrix} f(x_1, y_1) & \cdots & f(x_1, y_n) \\ \vdots & \ddots & \vdots \\ f(x_m, y_1) & \cdots & f(x_m, y_n) \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}.$$

Value

`outer1` and `outer2` return a matrix. `outer1_matvec` and `outer2_matvec` return a vector. See section "Outer" of the package vignette for details.

Examples

```
set.seed(1234)
f = function(x,y) { sum( (x - y)^2 ) }
X = matrix(rnorm(12), 6, 2)
Y = matrix(rnorm(10), 5, 2)
outer1(X, f)
outer2(X, Y, f)

a = rep(1, 6)
b = rep(1, 5)
outer1_matvec(X, f, a)
```

```
outer2_matvec(X, Y, f, b)
```

---

solve_cg *Iteratively Solve a Linear System with Conjugate Gradient*

Description

Solve the system $l(x) = b$ where $l(x)$ is a matrix-free representation of the linear operation Ax.

Usage

```
solve_cg(l, b, init, args)
```

Arguments

l	A linear transformation of x.
b	A vector.
init	Initial value of solution.
args	List of additional arguments from `cg_args`.

Value

A list with the form of a `solve_cg_result` described in section "Conjugate Gradient" of the package vignette.

Examples

```
set.seed(1234)

n = 8
idx_diag = cbind(1:n, 1:n)
idx_ldiag = cbind(2:n, 1:(n-1))
idx_udiag = cbind(1:(n-1), 2:n)
b = rep(1, n)

## Solution by explicit computation of solve(A, b)
A = matrix(0, n, n)
A[idx_diag] = 2
A[idx_ldiag] = 1
A[idx_udiag] = 1
solve(A, b)

## Solve iteratively with solve_cg
f = function(x) { A %*% x }
args = cg_args()
init = rep(0, n)
solve_cg(f, b, init, args)
```

univariate-optimization *Univariate Optimization*

Description

Univariate Optimization

Usage

```
goldensection(f, lower, upper, args)

optimize_brent(f, lower, upper, args)
```

Arguments

`f`	Function to optimize.
`lower`	Lower limit of search interval. Must be finite.
`upper`	Upper limit of search interval. Must be finite.
`args`	List of additional arguments from the function `optimize_args`.

Value

A list with the form of a `optimize_result` described in section "Univariate Optimization" of the package vignette.

Examples

```
f = function(x) { x^2 - 1 }
args = optimize_args()
goldensection(f, 0, 10, args)
optimize_brent(f, 0, 10, args)
```

which0 *Matrix Which Function*

Description

Matrix Which Function

Usage

```
which0(X, f)
```

Arguments

`X`	A matrix
`f`	A predicate to apply to each element of X.

Details

The `which` C++ functions are intended to operate like the following call in R.

```
which(f(X), arr.ind = TRUE) - 1
```

The R functions exposed here are specific to numeric-valued matrices, but the underlying C++ functions are intended to work with any type of Rcpp Matrix.

Value

A matrix with two columns. Each row contains a row and column index corresponding to an element of X that matches the criteria of f. See section "Which" of the package vignette for details.

Examples

```
X = matrix(1:12 / 6, nrow = 4, ncol = 3)
f = function(x) { x < 1 }
which0(X, f)
```

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