# Package 'pracma'

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R topics documented:
pracma-package
abm3pc
accumarray
agmean
aitken
akimaInterp
and, or
andrewsplot

angle	
approx_entropy	21
arclength	23
barylag	25
barylag2d	26
bisect	
bits	
blanks	
blkdiag	
brentDekker	
brown72	
broyden	
bsxfun	
bulirsch-stoer	
bvp	
cart2sph	
cd, pwd, what	
ceil	
charpoly	
chebApprox	
chebCoeff	
chebPoly	46
circlefit	47
clear, who(s), ver	49
clenshaw_curtis	50
combs	51
compan	51
complexstep	
cond	
conv	
cot,csc,sec, etc.	
cotes	
coth,csch,sech, etc.	
cranknic	
Cross	
crossn	
cubicspline	
curvefit	64
cutpoints	66
dblquad	67
deconv	69
deeve	70
deg2rad	71
detrend	71
deval	72
Diag	73
direct1d	74
disp,beep	76

distmat	76
$dot \ . \ . \ . \ . \ . \ . \ . \ . \ . \ $	78
eig	78
eigjacobi	79
einsteinF	80
ellipke,ellipj	82
eps	83
erf	84
errorbar	85
eta	86
euler_heun	87
expint	88
expm	90
eye	92
ezcontour,ezmesh	92
ezplot	94
ezpolar	95
fact	96
factors	97
fderiv	98
fibsearch	99
figure	100
findintervals	101
findmins	102
findpeaks	103
finds	104
$findzeros \dots \dots$	105
fletcher-powell	106
$flipdim \dots \dots$	108
$fminbnd \ \dots $	
fminsearch	110
$fnorm \ \dots $	
fornberg	113
$fplot \ \dots $	
fresnelS/C	115
fsolve	117
fzero	118
fzsolve	119
gammainc	120
$gammaz \ \dots $	121
gaussHermite	122
gaussLaguerre	124
gaussLegendre	125
gaussNewton	126
$gauss\_kronrod \dots \dots$	128
gcd, lcm	129
geomean, harmmean	130
goo median	121

givens	
gmres	. 133
golden_ratio	. 135
grad	. 136
gradient	. 137
gramSchmidt	
hadamard	. 139
halley	
hampel	
hankel	
hausdorff_dist	
hessian	
hilb	
histe	
histss	
hooke_jeeves	
horner	
householder	
humps	
hurstexp	
hypot	
ifft	
inpolygon	
integral	
integral2	
interp1	
interp2	
inv	
invlap  .  .  .  .  .  .  .  .  .	
invperm	
isempty	
isprime	
itersolve	
jacobian	
kriging	
kron	
L1linreg	. 176
laguerre	. 178
$lambertWp  \dots $	. 179
laplacian	. 180
lebesgue	. 182
legendre	. 183
line_integral	. 184
linprog	. 185
linspace	
logspace	
lsqlin	
lsqnonlin	

IU	. 195
magic	. 197
matlab	. 198
meshgrid	. 198
mexpfit	. 199
mldivide	. 201
mod, rem	. 202
Mode	. 203
moler	. 204
movavg	. 205
muller	. 203
nchoosek	. 208
ndims	. 208
nearest_spd	. 210
nelder_mead	. 211
neville	. 213
newmark	. 214
newtonHorner	. 215
newtonInterp	. 216
newtonRaphson	. 217
newtonsys	. 219
nextpow2	. 220
nile	. 221
nnz	. 222
Norm	. 223
normest	. 224
nthroot	. 225
nullspace	. 226
numderiv	. 227
numel	. 228
ode23	. 229
odregress	. 232
orth	. 234
pade	. 235
pascal	. 236
pchip	. 237
	. 237
peaks	
piecewise	
pinv	
plotyy	
polar	
Poly	
poly2str	
polyadd	
polyApprox	
polyarea	
polyder	250

polyfit	251
polyint	252
polylog	253
polymul	254
polypow	
1 71	256
polyval	257
pow2	
ppfit	
ppval	
primes	
procrustes	
psi	
qpspecial	
qrSolve	
quad	
quad2d	
quadec	
quadgk	
quadgr	
quadinf	
quadl	
quadv	
quiver	
rand	
randcomb	
randperm	
Rank	
rat	
ratinterp	284
rationalfit	285
rectint	287
refindall	288
regexp	289
regexprep	290
repmat	291
Reshape	292
ridders	292
rk4, rk4sys	294
rkf54	296
rmserr	298
romberg	
roots	
rortho	
rosser	
rot90	
rref	
runge	
101150	, U-F

Index

353

runs.test	5
savgol	6
segm_distance	8
segm_intersect	9
semilogx,semilogy	1
sigmoid	2
simpadpt	3
simpson2d	4
size	5
softline	6
sorting	7
sortrows	
spinterp	
sqrtm,rootm	2
squareform	
std	
std_err	6
steep_descent	
str2num	
strcat	
strcmp	
strfind	
strjust	
strrep	
strTrim	
subspace	
taylor	
tic,toc	
titanium	
Toeplitz	
Trace	
trapz	
tri	
trigApprox	2
trigPoly	_
triquad	5
trisolve	6
vander	
vectorfield	8
whittaker	
wilkinson	
zeta	1

8 pracma-package

pracma-package

Practical Numerical Math Routines

### Description

This package provides R implementations of more advanced functions in numerical analysis, with a special view on on optimization and time series routines. Uses Matlab/Octave function names where appropriate to simplify porting.

Some of these implementations are the result of courses on Scientific Computing ("Wissenschaftliches Rechnen") and are mostly intended to demonstrate how to implement certain algorithms in R/S. Others are implementations of algorithms found in textbooks.

#### **Details**

The package encompasses functions from all areas of numerical analysis, for example:

- Root finding and minimization of univariate functions, e.g. Newton-Raphson, Brent-Dekker, Fibonacci or 'golden ratio' search.
- Handling polynomials, including roots and polynomial fitting, e.g. Laguerre's and Muller's methods.
- Interpolation and function approximation, barycentric Lagrange interpolation, Pade and rational interpolation, Chebyshev or trigonometric approximation.
- Some special functions,
  - e.g. Fresnel integrals, Riemann's Zeta or the complex Gamma function, and Lambert's W computed iteratively through Newton's method.
- Special matrices, e.g. Hankel, Rosser, Wilkinson
- Numerical differentiation and integration,
   Richardson approach and "complex step" derivatives, adaptive Simpson and Lobatto integration and adaptive Gauss-Kronrod quadrature.
- Solvers for ordinary differential equations and systems,
   Euler-Heun, classical Runge-Kutta, ode23, or predictor-corrector method such as the Adams-Bashford-Moulton.
- Some functions from number theory, such as primes and prime factorization, extended Euclidean algorithm.
- Sorting routines, e.g. recursive quickstep.
- Several functions for string manipulation and regular search, all wrapped and named similar to their Matlab analogues.

It serves two main goals:

- Collecting R scripts that can be demonstrated in courses on 'Numerical Analysis' or 'Scientific Computing' using R/S as the chosen programming language.
- Wrapping functions with appropriate Matlab names to simplify porting programs from Matlab or Octave to R.

pracma-package 9

Providing an environment in which R can be used as a full-blown numerical computing system.

Besides that, many of these functions could be called in R applications as they do not have comparable counterparts in other R packages (at least at this moment, as far as I know).

All referenced books have been utilized in one way or another. Web links have been provided where reasonable.

#### Note

The following 220 functions are emulations of correspondingly named Matlab functions and bear the same signature as their Matlab cousins if possible:

```
accumarray, acot, acoth, acsc, acsch, and, angle, ans, arrayfun, asec, asech,
beep, blank, blkdiag, bsxfun,
cart2pol, cart2sph, cd, ceil, circshift, clear, compan, cond, conv,
cot, coth, cross, csc, csch, cumtrapz,
dblquad, deblank, deconv, deg2rad, detrend, deval, disp, dot,
eig, eigint, ellipj, ellipke, eps, erf, erfc, erfcinv, erfcx, erfi, erfinv,
errorbar, expint, expm, eye, ezcontour, ezmesh, ezplot, ezpolar,
fact, fftshift, figure, findpeaks, findstr, flipdim, fliplr, flipud,
fminbnd, fminsearch, fplot, fsolve, fzero,
gammainc, gcd, geomean, gmres, gradient,
hadamard, hankel, harmmean, hilb, histc, humps, hypot,
idivide, ifft, ifftshift, inpolygon, integral, integral2, integral3,
interp1, interp2, inv, isempty, isprime,
kron,
legendre, linprog, linspace, loglog, logm, logseq, logspace, lsqcurvefit,
lsqlin, lsqnonlin, lsqnonneg, lu,
magic, meshgrid, mkpp, mldivide, mod, mrdivide,
nchoosek, ndims, nextpow2, nnz, normest, nthroot, null, num2str, numel,
ode23, ones, or, orth,
pascal, pchip, pdist, pdist2, peaks, perms, piecewise, pinv, plotyy,
pol2cart, polar, polyfit, polyint, polylog, polyval, pow2, ppval,
primes, psi, pwd,
quad, quad2d, quadgk, quad1, quadprog, quadv, quiver,
rad2deg, randi, randn, randsample, rat, rats, regexp, regexpi,
regexpreg, rem, repmat, roots, rosser, rot90, rref, runge,
sec, sech, semilogx, semilogy, sinc, size, sortrows, sph2cart, sqrtm,
squareform, std, str2num, strcat, strcmp, strcmpi, strfind, strfindi,
strjust, strrep, subspace,
tic, toc, trapz, tril, trimmean, triplequad, triu,
vander, vectorfield, ver,
what, who, whos, wilkinson,
zeros, zeta
```

The following Matlab function names have been capitalized in 'pracma' to avoid shadowing functions from R base or one of its recommended packages (on request of Bill Venables and because of Brian Ripley's CRAN policies):

10 pracma-package

```
Diag, factos, finds, Fix, Imag, Lcm, Mode, Norm, nullspace (<- null), Poly, Rank, Real, Reshape, strTrim, Toeplitz, Trace, uniq (<- unique).
```

To use "ans" instead of "ans()" – as is common practice in Matlab – type (and similar for other Matlab commands):

```
makeActiveBinding("ans", function() .Last.value, .GlobalEnv)
makeActiveBinding("who", who(), .GlobalEnv)
```

#### Author(s)

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#### References

Abramowitz, M., and I. A. Stegun (1972). Handbook of Mathematical Functions (with Formulas, Graphs, and Mathematical Tables). Dover, New York. http://www.nr.com/aands/.

Arndt, J. (2010). Matters Computational: Ideas, Algorithms, Source Code. Springer-Verlag, Berlin Heidelberg Dordrecht. FXT: a library of algorithms: http://www.jjj.de/fxt/.

Cormen, Th. H., Ch. E. Leiserson, and R. L. Rivest (2009). Introduction to Algorithms. Third Edition, The MIT Press, Cambridge, MA.

Encyclopedia of Mathematics (2012). Editor-in-Chief: Ulf Rehmann. http://www.encyclopediaofmath.org/.

Gautschi, W. (1997). Numerical Analysis: An Introduction. Birkhaeuser, Boston.

Gentle, J. E. (2009). Computational Statistics. Springer Science+Business Media LCC, New York.

Hazewinkel, M., Editor (2002). Encyclopaedia of Mathematics. Springer-Verlag, Berlin Heidelberg New York. http://eom.springer.de/.

MathWorld.com (2011). Matlab Central: http://www.mathworks.com/matlabcentral/. Mathtools.net: http://www.mathtools.net/.

NIST: National Institute of Standards and Technology. Olver, F. W. J., et al. (2010). NIST Handbook of Mathematical Functions. Cambridge University Press. Internet: NIST Digital Library of Mathematical Functions, http://dlmf.nist.gov/; Dictionary of Algorithms and Data Structures, http://xlinux.nist.gov/dads/; Guide to Available Mathematical Software, http://gams.nist.gov/

Press, W. H., S. A. Teukolsky, W. T Vetterling, and B. P. Flannery (2007). Numerical Recipes: The Art of Numerical Computing. Third Edition, incl. Numerical Recipes Software, Cambridge University Press, New York. http://www.nrbook.com/a/bookcpdf.php [chapters], or http://apps.nrbook.com/c/index.html [pages].

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

Skiena, St. S. (2008). The Algorithm Design Manual. Second Edition, Springer-Verlag, London. The Stony Brook Algorithm Repository: http://www.cs.sunysb.edu/~algorith/.

Stoer, J., and R. Bulirsch (2002). Introduction to Numerical Analysis. Third Edition, Springer-Verlag, New York.

abm3pc 11

Strang, G. (2007). Computational Science and Engineering. Wellesley-Cambridge Press. Matlab Codes: http://www-math.mit.edu/cse/

Weisstein, E. W. (2003). CRC Concise Encyclopedia of Mathematics. Second Edition, Chapman & Hall/CRC Press. Wolfram MathWorld: http://mathworld.wolfram.com/.

Zhang, S., and J. Jin (1996). Computation of Special Functions. John Wiley & Sons. http://jin.ece.illinois.edu/specfunc.html

#### See Also

The R package 'matlab' contains some of the basic routines from Matlab, but unfortunately not any of the higher math routines.

# **Examples**

```
## Not run:
## See examples in the help files for all functions.
## End(Not run)
```

abm3pc

Adams-Bashford-Moulton

### **Description**

Third-order Adams-Bashford-Moulton predictor-corrector method.

### Usage

```
abm3pc(f, a, b, y0, n = 50, ...)
```

### **Arguments**

```
f function in the differential equation y' = f(x, y).

a, b endpoints of the interval.

y0 starting values at point a.

n the number of steps from a to b.

... additional parameters to be passed to the function.
```

# Details

Combined Adams-Bashford and Adams-Moulton (or: multi-step) method of third order with corrections according to the predictor-corrector approach.

#### Value

List with components x for grid points between a and b and y a vector y the same length as x; additionally an error estimation est.error that should be looked at with caution.

12 accumarray

# Note

This function serves demonstration purposes only.

#### References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

#### See Also

```
rk4, ode23
```

# **Examples**

```
## Attempt on a non-stiff equation
# y' = y^2 - y^3, y(0) = d, 0 <= t <= 2/d, d = 0.01
f <- function(t, y) y^2 - y^3
d <- 1/250
abm1 <- abm3pc(f, 0, 2/d, d, n = 1/d)
abm2 <- abm3pc(f, 0, 2/d, d, n = 2/d)
## Not run:
plot(abm1$x, abm1$y, type = "1", col = "blue")
lines(abm2$x, abm2$y, type = "1", col = "red")
grid()
## End(Not run)</pre>
```

accumarray

Accumulate Vector Elements

# Description

accumarray groups elements from a data set and applies a function to each group.

# Usage

```
accumarray(subs, val, sz = NULL, func = sum, fillval = 0)
uniq(a, first = FALSE)
```

### **Arguments**

subs	vector or matrix of positive integers, used as indices for the result vector.
val	numerical vector.
SZ	size of the resulting array.
func	function to be applied to a vector of numbers.
fillval	value used to fill the array when there are no indices pointing to that component.
а	numerical vector.
first	logical, shall the first or last element encountered be used.

accumarray 13

### **Details**

A <- accumarray(subs, val) creates an array A by accumulating elements of the vector val using the lines of subs as indices and applying func to that accumulated vector. The size of the array can be predetermined by the size vector sz.

A = uniq(a) returns a vector b identical to unique(a) and two other vectors of indices m and n such that b == a[m] and a == b[n].

#### Value

accumarray returns an array of size the maximum in each column of subs, or by sz. uniq returns a list with components

```
b vector of unique elements of a.m vector of indices such that b = a[m]n vector of indices such that a = b[n]
```

#### Note

The Matlab function accumarray can also handle sparse matrices.

#### See Also

unique

```
## Examples for accumarray
val = 101:105
subs = as.matrix(c(1, 2, 4, 2, 4))
accumarray(subs, val)
# [101; 206; 0; 208]
val = 101:105
subs <- matrix(c(1,2,2,2,2,1,1,3,1,3,1,2,2,2,2), ncol = 3)
accumarray(subs, val)
# , , 1
# [,1] [,2] [,3]
# [1,] 101
                   0
# [2,]
         0
# , , 2
# [,1] [,2] [,3]
                   0
# [1,]
       0
              0 208
# [2,] 206
val = 101:106
subs <- matrix(c(1, 2, 1, 2, 3, 1, 4, 1, 4, 4, 4, 1), ncol = 2, byrow = TRUE)
accumarray(subs, val, func = function(x) sum(diff(x)))
# [,1] [,2] [,3] [,4]
#[1,] 0 1
                   0
                        0
         0
              0
# [2,]
                   0
                        0
```

14 agmean

```
# [3,]
         0
# [4,]
val = 101:105
subs = matrix(c(1, 1, 2, 1, 2, 3, 2, 1, 2, 3), ncol = 2, byrow = TRUE)
accumarray(subs, val, sz = c(3, 3), func = max, fillval = NA)
# [,1] [,2] [,3]
# [1,] 101
                 NA
            NA
# [2,] 104
            NA 105
# [3,]
            NA
                NA
       NA
## Examples for uniq
a <- c(1, 1, 5, 6, 2, 3, 3, 9, 8, 6, 2, 4)
A <- uniq(a); A
# A$b 1 5 6 2 3 9 8 4
# A$m 2 3 10 11 7 8 9 12
# A$n 1 1 2 3 4 5 5 6 7 3 4 8
A <- uniq(a, first = TRUE); A
# A$m 1 3 4 5 6 8 9 12
## Example: Subset sum problem
# Distribution of unique sums among all combinations of a vectors.
allsums <- function(a) {</pre>
   S <- c(); C <- c()
   for (k in 1:length(a)) {
       U \leftarrow uniq(c(S, a[k], S + a[k]))
       S <- U$b
       C \leftarrow accumarray(U$n, c(C, 1, C))
   o <- order(S); S <- S[o]; C <- C[o]</pre>
   return(list(S = S, C = C))
}
A \leftarrow allsums(seq(1, 9, by=2)); A
# A$S 1 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 24 25
```

agmean

Arithmetic-geometric Mean

# **Description**

The arithmetic-geometric mean of real or complex numbers.

# Usage

```
agmean(a, b)
```

### **Arguments**

a, b vectors of real or complex numbers of the same length (or scalars).

agmean 15

### **Details**

The arithmetic-geometric mean is defined as the common limit of the two sequences  $a_{n+1} = (a_n + b_n)/2$  and  $b_{n+1} = \sqrt{(a_n b_n)}$ .

When used for negative or complex numbers, the complex square root function is applied.

### Value

Returns a list with components: agm a vector of arithmetic-geometric means, component-wise, niter the number of iterations, and prec the overall estimated precision.

#### Note

Gauss discovered that elliptic integrals can be effectively computed via the arithmetic-geometric mean (see example below), for example:

$$\int_0^{\pi/2} \frac{dt}{\sqrt{1 - m^2 sin^2(t)}} = \frac{(a+b)\pi}{4 \cdot agm(a,b)}$$

where m = (a - b)/(a + b)

#### References

http://mathworld.wolfram.com/Arithmetic-GeometricMean.html

#### See Also

Arithmetic, geometric, and harmonic mean.

```
## Accuracy test: Gauss constant
1/agmean(1, sqrt(2)) agm - 0.834626841674073186 # 1.11e-16 < eps = 2.22e-16
## Example: Approximate elliptic integral
N <- 20
m \leftarrow seq(0, 1, len = N+1)[1:N]
E <- numeric(N)</pre>
for (i in 1:N) {
    f \leftarrow function(t) \frac{1}{sqrt(1 - m[i]^2 * sin(t)^2)}
    E[i] \leftarrow quad(f, 0, pi/2)
}
A <- numeric(2*N-1)
b <- a * (1-m) / (m+1)
## Not run:
plot(m, E, main = "Elliptic Integrals vs. arith.-geom. Mean")
lines(m, (a+b)*pi / 4 / agmean(a, b)$agm, col="blue")
grid()
## End(Not run)
```

16 aitken

	ken	

Aitken' Method

# Description

Aitken's acceleration method.

### Usage

```
aitken(f, x0, nmax = 12, tol = 1e-8, ...)
```

### **Arguments**

f Function with a fixpoint.

x0 Starting value.

nmax Maximum number of iterations.

tol Relative tolerance.

... Additional variables passed to f.

### **Details**

Aitken's acceleration method, or delta-squared process, is used for accelerating the rate of convergence of a sequence (from linear to quadratic), here applied to the fixed point iteration scheme of a function.

# Value

The fixpoint (as found so far).

### Note

Sometimes used to accerate Newton-Raphson (Steffensen's method).

### References

Quarteroni, A., and F. Saleri (2006). Scientific Computing with Matlab and Octave. Second Edition, Springer-Verlag, Berlin Heidelberg.

#### See Also

1ambertWp

```
# Find a zero of f(x) = cos(x) - x*exp(x)
# as fixpoint of phi(x) = x + (cos(x) - x*exp(x))/2
phi <- function(x) x + (cos(x) - x*exp(x))/2
aitken(phi, 0) #=> 0.5177574
```

akimaInterp 17

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Univariate Akima Interpolation

### Description

Interpolate smooth curve through given points on a plane.

# Usage

```
akimaInterp(x, y, xi)
```

### **Arguments**

x, y x/y-coordinates of (irregular) grid points defining the curve.

xi x-coordinates of points where to interpolate.

### **Details**

Implementation of Akima's univariate interpolation method, built from piecewise third order polynomials. There is no need to solve large systems of equations, and the method is therefore computationally very efficient.

### Value

Returns the interpolated values at the points xi as a vector.

### Note

There is also a 2-dimensional version in package 'akima'.

### Author(s)

Matlab code by H. Shamsundar under BSC License; re-implementation in R by Hans W Borchers.

### References

Akima, H. (1970). A New Method of Interpolation and Smooth Curve Fitting Based on Local Procedures. Journal of the ACM, Vol. 17(4), pp 589-602.

Hyman, J. (1983). Accurate Monotonicity Preserving Cubic Interpolation. SIAM J. Sci. Stat. Comput., Vol. 4(4), pp. 645-654.

Akima, H. (1996). Algorithm 760: Rectangular-Grid-Data Surface Fitting that Has the Accurancy of a Bicubic Polynomial. ACM TOMS Vol. 22(3), pp. 357-361.

Akima, H. (1996). Algorithm 761: Scattered-Data Surface Fitting that Has the Accuracy of a Cubic Polynomial. ACM TOMS, Vol. 22(3), pp. 362-371.

and, or

### See Also

```
kriging, akima::aspline, akima::interp
```

# **Examples**

```
x \leftarrow c(0, 2, 3, 5, 6, 8, 9, 11, 12, 14, 15)
y \leftarrow c(10, 10, 10, 10, 10, 10, 10.5, 15, 50, 60, 85)
                        # 12.0 12.5
                                                                 14.0
xs <- seq(12, 14, 0.5)
                                            13.0
                                                        13.5
ys <- akimaInterp(x, y, xs) # 50.0 54.57405 54.84360 55.19135 60.0
xs; ys
## Not run:
plot(x, y, col="blue", main = "Akima Interpolation")
xi <- linspace(0,15,51)
yi <- akimaInterp(x, y, xi)</pre>
lines(xi, yi, col = "darkred")
grid()
## End(Not run)
```

and, or

Logical AND, OR (Matlab Style)

### **Description**

```
and(1, k) resp. or(1, k) the same as (1 & k) + \theta resp. (1 | k) + \theta.
```

# Usage

```
and(1, k) or(1, k)
```

### **Arguments**

1, k Arrays.

# **Details**

Performs a logical operation of arrays 1 and k and returns an array containing elements set to either 1 (TRUE) or 0 (FALSE), that is in Matlab style.

### Value

Logical vector.

andrewsplot 19

### **Examples**

andrewsplot

Andrews' Curves

# **Description**

Plots Andrews' curves in cartesian or polar coordinates.

### Usage

```
andrewsplot(A, f, style = "pol", scaled = FALSE, npts = 101)
```

# Arguments

Α	numeric matrix with at least two columns.
f	factor or integer vector with nrow(A) elements.
style	character variable, only possible values 'cart' or 'pol'.
scaled	logical; if true scales each column to have mean $0$ and standard deviation $1$ (not yet implemented).
npts	number of points to plot.

# Details

andrewsplot creates an Andrews plot of the multivariate data in the matrix A, assigning different colors according to the factor or integer vector f.

Andrews' plot represent each observation (row) by a periodic function over the interval [0, 2\*pi]. This function for the i-th observation is defined as ...

The plot can be seen in cartesian or polar coordinates — the latter seems appropriate as all these functions are periodic.

### Value

Generates a plot, no return value.

20 angle

### Note

Please note that a different ordering of the columns will result in quite different functions and overall picture.

There are variants utilizing principal component scores, in order of decreasing eigenvalues.

# References

R. Khattree and D. N. Naik (2002). Andrews PLots for Multivariate Data: Some New Suggestions and Applications. Journal of Statistical Planning and Inference, Vol. 100, No. 2, pp. 411–425.

### See Also

```
polar, andrews::andrews
```

### **Examples**

```
## Not run:
data(iris)
s <- sample(1:4, 4)
A <- as.matrix(iris[, s])
f <- as.integer(iris[, 5])
andrewsplot(A, f, style = "pol")
## End(Not run)</pre>
```

angle

Basic Complex Functions

# Description

Basic complex functions (Matlab style)

### Usage

```
Real(z)
Imag(z)
angle(z)
```

### **Arguments**

z Vector or matrix of real or complex numbers

### **Details**

These are just Matlab names for the corresponding functions in R. The angle function is simply defined as atan2(Im(z), Re(z)).

approx\_entropy 21

# Value

returning real or complex values; angle returns in radians.

# Note

The true Matlab names are real, imag, and conj, but as real was taken in R, all these beginnings are changed to capitals.

The function Mod has no special name in Matlab; use abs() instead.

# See Also

```
Mod, abs
```

# **Examples**

```
z <- c(0, 1, 1+1i, 1i)
Real(z)  # Re(z)
Imag(z)  # Im(z)
Conj(z)  # Conj(z)
abs(z)  # Mod(z)
angle(z)</pre>
```

approx\_entropy

Approximate and Sample Entropy

# Description

Calculates the approximate or sample entropy of a time series.

# Usage

```
approx_entropy(ts, edim = 2, r = 0.2*sd(ts), elag = 1) sample_entropy(ts, edim = 2, r = 0.2*sd(ts), tau = 1)
```

# Arguments

ts	a time series.
edim	the embedding dimension, as for chaotic time series; a preferred value is 2.
r	filter factor; work on heart rate variability has suggested setting r to be $0.2$ times the standard deviation of the data.
elag	embedding lag; defaults to 1, more appropriately it should be set to the smallest lag at which the autocorrelation function of the time series is close to zero. (At the moment it cannot be changed by the user.)
tau	delay time for subsampling, similar to elag.

22 approx\_entropy

#### **Details**

Approximate entropy was introduced to quantify the the amount of regularity and the unpredictability of fluctuations in a time series. A low value of the entropy indicates that the time series is deterministic; a high value indicates randomness.

Sample entropy is conceptually similar with the following differences: It does not count self-matching, and it does not depend that much on the length of the time series.

#### Value

The approximate, or sample, entropy, a scalar value.

#### Note

There exists a translation of the Kaplan code to R by Ben Bolker, see <a href="http://www.macalester.edu/~kaplan/hrv/doc/funs/apen.html">http://www.macalester.edu/~kaplan/hrv/doc/funs/apen.html</a>.

This code here derives from Matlab versions at Mathwork's File Exchange, "Fast Approximate Entropy" and "Sample Entropy" by Kijoon Lee under BSD license.

#### References

Pincus, S.M. (1991). Approximate entropy as a measure of system complexity. Proc. Natl. Acad. Sci. USA, Vol. 88, pp. 2297–2301.

Kaplan, D., M. I. Furman, S. M. Pincus, S. M. Ryan, L. A. Lipsitz, and A. L. Goldberger (1991). Aging and the complexity of cardiovascular dynamics, Biophysics Journal, Vol. 59, pp. 945–949.

Yentes, J.M., N. Hunt, K.K. Schmid, J.P. Kaipust, D. McGrath, N. Stergiou (2012). The Appropriate use of approximate entropy and sample entropy with short data sets. Ann. Biomed. Eng.

### See Also

RHRV::CalculateApEn

```
ts <- rep(61:65, 10)
approx_entropy(ts, edim = 2)
                                                  # -0.000936195
sample_entropy(ts, edim = 2)
                                                  # 0
set.seed(8237)
approx_entropy(rnorm(500), edim = 2)
                                                  # 1.48944 high, random
approx_entropy(sin(seq(1,100,by=0.2)), edim = 2) # 0.22831 low, deterministic
sample_entropy(sin(seq(1,100,by=0.2)), edim = 2) # 0.2359326
## Not run: (Careful: This will take several minutes.)
# generate simulated data
N \leftarrow 1000; t \leftarrow 0.001*(1:N)
sint <- sin(2*pi*10*t); sd1 <- sd(sint)
                                              # sine curve
chirpt <- sint + 0.1*whitet; sd2 <- sd(chirpt) # chirp signal</pre>
whitet <- rnorm(N); sd3 <- sd(whitet) # white noise</pre>
```

arclength 23

```
# calculate approximate entropy
rnum <- 30; result <- zeros(3, rnum)</pre>
for (i in 1:rnum) {
    r <- 0.02 * i
    result[1, i] <- approx_entropy(sint, 2, r*sd1)</pre>
    result[2, i] <- approx_entropy(chirpt, 2, r*sd2)</pre>
    result[3, i] <- approx_entropy(whitet, 2, r*sd3)</pre>
}
# plot curves
r <- 0.02 * (1:rnum)
plot(c(0, 0.6), c(0, 2), type="n",
      xlab = "", ylab = "", main = "Approximate Entropy")
points(r, result[1, ], col="red"); lines(r, result[1, ], col="red")
points(r, result[2, ], col="green"); lines(r, result[2, ], col="green")
points(r, result[3, ], col="blue"); lines(r, result[3, ], col="blue")
grid()
## End(Not run)
```

arclength

Arc Length of a Curve

### **Description**

Calculates the arc length of a parametrized curve.

#### **Usage**

```
arclength(f, a, b, nmax = 20, tol = 1e-05, ...)
```

#### **Arguments**

f parametrization of a curve in n-dim. space.

a,b begin and end of the parameter interval.

nmax maximal number of iterations.

tol relative tolerance requested.

... additional arguments to be passed to the function.

# Details

Calculates the arc length of a parametrized curve in R^n. It applies Richardson's extrapolation by refining polygon approximations to the curve.

The parametrization of the curve must be vectorized: if t-->F(t) is the parametrization, F(c(t1,t1,...)) must return c(F(t1),F(t2),...).

Can be directly applied to determine the arc length of a one-dimensional function f:R-->R by defining F (if f is vectorized) as F:t-->c(t,f(t)).

24 arclength

#### Value

Returns a list with components length the calculated arc length, niter the number of iterations, and rel.err the relative error generated from the extrapolation.

#### Note

If by chance certain equidistant points of the curve lie on a straight line, the result may be wrong, then use polylength below.

#### Author(s)

HwB <hwborchers@googlemail.com>

#### See Also

```
poly_length
```

```
## Example: parametrized 3D-curve with t in 0..3*pi
f <- function(t) c(sin(2*t), cos(t), t)
arclength(f, 0, 3*pi)
# $length: 17.22203
                                 # true length 17.222032...
## Example: length of the sine curve
f <- function(t) c(t, sin(t))</pre>
arclength(f, 0, pi)
                                 # true length 3.82019...
## Example: Length of an ellipse with axes a = 1 and b = 0.5
# parametrization x = a*cos(t), y = b*sin(t)
a <- 1.0; b <- 0.5
f <- function(t) c(a*cos(t), b*sin(t))</pre>
L \leftarrow \operatorname{arclength}(f, 0, 2*pi, tol = 1e-10)
                                            #=> 4.84422411027
# compare with elliptic integral of the second kind
e <- sqrt(1 - b^2/a^2)
                                              # ellipticity
L \leftarrow 4 * a * ellipke(e^2)$e
                                              #=> 4.84422411027
## Not run:
## Example: oscillating 1-dimensional function (from 0 to 5)
f \leftarrow function(x) x * cos(0.1*exp(x)) * sin(0.1*pi*exp(x))
F <- function(t) c(t, f(t))
L < - arclength(F, 0, 5, tol = 1e-12, nmax = 25)
print(L$length, digits = 16)
# [1] 82.81020372882217
                                 # true length 82.810203728822172...
# Split this computation in 10 steps (run time drops from 2 to 0.2 secs)
L <- 0
for (i in 1:10)
L \leftarrow L + arclength(F, (i-1)*0.5, i*0.5, tol = 1e-10)$length
print(L, digits = 16)
# [1] 82.81020372882216
```

barylag 25

```
# Alternative calculation of arc length
f1 <- function(x) sqrt(1 + complexstep(f, x)^2)
L1 <- quadgk(f1, 0, 5, tol = 1e-14)
print(L1, digits = 16)
# [1] 82.81020372882216
## End(Not run)</pre>
```

barylag

Barycentric Lagrange Interpolation

# **Description**

Barycentric Lagrange interpolation in one dimension.

# Usage

```
barylag(xi, yi, x)
```

# Arguments

```
xi, yix- and y-coordinates of supporting nodes.xx-coordinates of interpolation points.
```

### **Details**

barylag interpolates the given data using the barycentric Lagrange interpolation formula (vectorized to remove all loops).

### Value

Values of interpolated data at points x.

### Note

Barycentric interpolation is preferred because of its numerical stability.

### References

Berrut, J.-P., and L. Nick Trefethen (2004). "Barycentric Lagrange Interpolation". SIAM Review, Vol. 46(3), pp.501–517.

# See Also

Lagrange or Newton interpolation.

26 barylag2d

### **Examples**

```
## Generates an example with plot.
   fun --- function that shall be 'approximated'
   a, b --- interval [a, b] to be used for the example
        --- number of supporting nodes
         --- number of interpolation points
# Output
   plot of function, interpolation, and nodes
   return value is NULL (invisible)
## Not run:
barycentricExample <- function(fun, a, b, n, m)</pre>
xi \leftarrow seq(a, b, len=n)
yi <- fun(xi)</pre>
x <- seq(a, b, len=m)
y <- barylag(xi, yi, x)
plot(xi, yi, col="red", xlab="x", ylab="y",
main="Example of barycentric interpolation")
lines(x, fun(x), col="yellow", lwd=2)
lines(x, y, col="darkred")
grid()
}
barycentricExample(sin, -pi, pi, 11, 101) # good interpolation
barycentricExample(runge, -1, 1, 21, 101) # bad interpolation
## End(Not run)
```

barylag2d

2-D Barycentric Lagrange Interpolation

# **Description**

Two-dimensional barycentric Lagrange interpolation.

# Usage

```
barylag2d(F, xn, yn, xf, yf)
```

# **Arguments**

F matrix representing values of a function in two dimensions.

xn, yn x- and y-coordinates of supporting nodes.

xf, yf x- and y-coordinates of an interpolating grid..

barylag2d 27

### **Details**

Well-known Lagrange interpolation using barycentric coordinates, here extended to two dimensions. The function is completely vectorized.

x-coordinates run downwards in F, y-coordinates to the right. That conforms to the usage in image or contour plots, see the example below.

#### Value

Matrix of size length(xf)-by-length(yf) giving the interpolated values at all the grid points (xf, yf).

### Note

Copyright (c) 2004 Greg von Winckel of a Matlab function under BSD license; translation to R by Hans W Borchers with permission.

#### References

Berrut, J.-P., and L. Nick Trefethen (2004). "Barycentric Lagrange Interpolation". SIAM Review, Vol. 46(3), pp.501–517.

#### See Also

```
interp2, barylag
```

```
## Example from R-help
xn \leftarrow c(4.05, 4.10, 4.15, 4.20, 4.25, 4.30, 4.35)
yn <- c(60.0, 67.5, 75.0, 82.5, 90.0)
foo <- matrix(c(</pre>
        -137.8379, -158.8240, -165.4389, -166.4026, -166.2593,
        -152.1720, -167.3145, -171.1368, -170.9200, -170.4605,
        -162.2264, -172.5862, -174.1460, -172.9923, -172.2861,
        -168.7746, -175.2218, -174.9667, -173.0803, -172.1853,
        -172.4453, -175.7163, -174.0223, -171.5739, -170.5384,
        -173.7736, -174.4891, -171.6713, -168.8025, -167.6662,
        -173.2124, -171.8940, -168.2149, -165.0431, -163.8390),
            nrow = 7, ncol = 5, byrow = TRUE)
xf <- c(4.075, 4.1)
yf <- c(63.75, 67.25)
barylag2d(foo, xn, yn, xf, yf)
# -156.7964 -163.1753
# -161.7495 -167.0424
# Find the minimum of the underlying function
bar <- function(xy) barylag2d(foo, xn, yn, xy[1], xy[2])</pre>
optim(c(4.25, 67.5), bar) # "Nelder-Mead"
# $par
# 4.230547 68.522747
# $value
```

28 bisect

```
# -175.7959

## Not run:
# Image and contour plots
image(xn, yn, foo)
contour(xn, yn, foo, col="white", add = TRUE)
xs <- seq(4.05, 4.35, length.out = 51)
ys <- seq(60.0, 90.0, length.out = 51)
zz <- barylag2d(foo, xn, yn, xs, ys)
contour(xs, ys, zz, nlevels = 20, add = TRUE)
contour(xs, ys, zz, levels=c(-175, -175.5), add = TRUE)
points(4.23, 68.52)
## End(Not run)</pre>
```

bisect

Rootfinding Through Bisection

### **Description**

Finding roots of univariate functions in bounded intervals.

# Usage

```
bisect(f, a, b, maxiter = 100, tol = NA)
regulaFalsi(f, a, b, maxiter = 100, tol = .Machine$double.eps^0.5)
```

### Arguments

f Function or its name as a string.

a, b interval end points.

maxiter maximum number of iterations; default 100.

tol absolute tolerance; default eps^(1/2)

#### **Details**

"Bisection" is a well known root finding algorithms for real, univariate, continuous functions. Bisection works in any case if the function has opposite signs at the endpoints of the interval.

bisect stops when floating point precision is reached, attaching a tolerance is no longer needed. This version is trimmed for exactness, not speed. Special care is taken when 0.0 is a root of the function. Argument 'tol' is deprecated and not used anymore.

"Regula falsi" combines bisection and secant methods. The so-called 'Illinois' improvement is used.

#### Value

Return a list with components root, f.root, the function value at the found root, iter, the number of iterations done, and root, and the estimated accuracy estim.prec

bits 29

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

```
ridders
```

### **Examples**

```
bisect(sin, 3.0, 4.0)
# $root $f.root $ite
# 3.1415926536 1.2246467991e-16 52
                                        $iter
                                                $estim.prec
                                                4.4408920985e-16
bisect(sin, -1.0, 1.0)
# $root
                   $f.root
                                        $iter
                                                $estim.prec
# 0
                    0
# Legendre polynomial of degree 5
lp5 <- c(63, 0, -70, 0, 15, 0)/8
f \leftarrow function(x) polyval(lp5, x)
bisect(f, 0.6, 1) # 0.9061798453
                                            correct to 15 decimals
regulaFalsi(f, 0.6, 1) # 0.9061798459
                                            correct to 10 decimals
```

bits

Binary Representation

# Description

Literal bit representation.

### Usage

```
bits(x, k = 54, pos_sign = FALSE, break0 = FALSE)
```

# Arguments

```
    x a positive or negative floating point number.
    k number of binary digits after the decimal point
    pos_sign logical; shall the '+' sign be included.
    break0 logical; shall trailing zeros be included.
```

### **Details**

The literal bit/binary representation of a floating point number is computed by subtracting powers of 2.

30 blanks

# Value

Returns a string containing the binary representation.

### See Also

```
nextpow2
```

# **Examples**

blanks

String of Blank Carakters

# Description

Create a string of blank characters.

# Usage

blanks(n)

# **Arguments**

n

integer greater or equal to 0.

### **Details**

blanks(n) is a string of n blanks.

# Value

String of n blanks.

### See Also

deblank

# **Examples**

blanks(6)

blkdiag 31

blkdiag

Block Diagonal Matrix

# **Description**

Build a block diagonal matrix.

# Usage

```
blkdiag(...)
```

# Arguments

. . . sequence of non-empty, numeric matrices

### **Details**

Generate a block diagonal matrix from A, B, C, .... All the arguments must be numeric and non-empty matrices.

### Value

a numeric matrix

### Note

Vectors as input have to be converted to matrices before. Note that as.matrix(v) with v a vector will generate a column vector; use matrix(v, nrow=1) if a row vector is intended.

# See Also

Diag

```
a1 <- matrix(c(1,2), 1)
a2 <- as.matrix(c(1,2))
blkdiag(a1, diag(1, 2, 2), a2)
```

32 brentDekker

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Brent-Dekker Root Finding Algorithm

# **Description**

Find root of continuous function of one variable.

### Usage

```
brentDekker(f, a, b, maxiter = 100, tol = .Machine$double.eps^0.75)
brent(f, a, b, maxiter = 100, tol = .Machine$double.eps^0.75)
```

### **Arguments**

f function whose root is to be found.

a, b left and right end points of an interval; function values need to be of different

sign at the endpoints.

maxiter maximum number of iterations.

tol relative tolerance.

#### **Details**

brentDekker implements a version of the Brent-Dekker algorithm, a well known root finding algorithms for real, univariate, continuous functions. The Brent-Dekker approach is a clever combination of secant and bisection with quadratic interpolation.

brent is simply an alias for brentDekker.

### Value

brent returns a list with

root location of the root.

f.root funtion value at the root.

f.calls number of function calls.

estim.prec estimated relative precision.

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

```
ridders, newtonRaphson
```

brown72 33

# **Examples**

```
# Legendre polynomial of degree 5
lp5 <- c(63, 0, -70, 0, 15, 0)/8
f <- function(x) polyval(lp5, x)
brent(f, 0.6, 1)  # 0.9061798459 correct to 10 places</pre>
```

brown72

Brownian Motion

# Description

The Brown72 data set represents a fractal Brownian motion with a prescribed Hurst exponent 0.72.

# Usage

```
data(brown72)
```

# **Format**

The format is: one column.

### **Details**

"Estimating the Hurst exponent for a data set provides a measure of whether the data is a pure random walk or has underlying trends. Brownian walks can be generated from a defined Hurst exponent."

### **Source**

http://www.bearcave.com/misl/misl\_tech/wavelets/hurst/

```
## Not run:
data(brown72)
plot(brown72, type = "1", col = "blue")
grid()
## End(Not run)
```

34 broyden

broyden	Broyden's Method	

### **Description**

Broyden's method for the numerical solution of nonlinear systems of n equations in n variables.

### Usage

# **Arguments**

Ffun	n functions of n variables.
x0	Numeric vector of length n.
J0	Jacobian of the function at x0.
	additional parameters passed to the function.
maxiter	Maximum number of iterations.
tol	Tolerance, relative accuracy.

### **Details**

F as a function must return a vector of length n, and accept an n-dim. vector or column vector as input.

Broyden's method computes the Jacobian and its inverse only at the first iteration, and does a rankone update thereafter, applying the so-called Sherman-Morrison formula that computes the inverse of the sum of an invertible matrix A and the dyadic product, uv', of a column vector u and a row vector v'.

### Value

List with components: zero the best root found so far, fnorm the square root of sum of squares of the values of f, and niter the number of iterations needed.

### Note

Applied to a system of n linear equations it will stop in 2n steps

# References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

#### See Also

```
newtonsys, fsolve
```

bsxfun 35

### **Examples**

```
## Example from Quarteroni & Saleri
F1 \leftarrow function(x) c(x[1]^2 + x[2]^2 - 1, sin(pi*x[1]/2) + x[2]^3)
broyden(F1, x0 = c(1, 1))
# zero: 0.4760958 -0.8793934; fnorm: 9.092626e-09; niter: 13
F <- function(x) {
    x1 \leftarrow x[1]; x2 \leftarrow x[2]; x3 \leftarrow x[3]
    as.matrix(c(x1^2 + x2^2 + x3^2 - 1)
                x1^2 + x3^2 - 0.25,
                x1^2 + x2^2 - 4*x3, ncol = 1
}
x0 <- as.matrix(c(1, 1, 1))
broyden(F, x0)
# zero: 0.4407629 0.8660254 0.2360680; fnorm: 1.34325e-08; niter: 8
## Find the roots of the complex function sin(z)^2 + sqrt(z) - log(z)
F2 <- function(x) {
    z <- x[1] + x[2]*1i
    fz \leftarrow \sin(z)^2 + \operatorname{sqrt}(z) - \log(z)
    c(Re(fz), Im(fz))
broyden(F2, c(1, 1))
# zero 0.2555197 0.8948303 , i.e. z0 = 0.2555 + 0.8948i
# fnorm 7.284374e-10
# niter 13
## Two more problematic examples
F3 <- function(x)
        c(2*x[1] - x[2] - exp(-x[1]), -x[1] + 2*x[2] - exp(-x[2]))
broyden(F3, c(0, 0))
# $zero 0.5671433 \ 0.5671433 \ # x = exp(-x)
F4 <- function(x) # Dennis Schnabel
        c(x[1]^2 + x[2]^2 - 2, exp(x[1] - 1) + x[2]^3 - 2)
broyden(F4, c(2.0, 0.5), maxiter = 100)
```

bsxfun

Elementwise Function Application (Matlab Style)

# Description

Apply a binary function elementwise.

# Usage

```
bsxfun(func, x, y)
arrayfun(func, ...)
```

36 bulirsch-stoer

### **Arguments**

func	function with two or more input parameters.
x, y	two vectors, matrices, or arrays of the same size.
	list of arrays of the same size.

#### **Details**

bsxfun applies element-by-element a binary function to two vectors or matrices of the same size. arrayfun applies func to each element of the arrays and returns an array of the same size.

### Value

The result will be a vector or matrix of the same size as x, y.

### Note

The underlying function mapply can be applied in a more general setting with many function parameters:

```
mapply(f, x, y, z, ...)
```

but the array structure will not be preserved in this case.

### See Also

Vectorize

# **Examples**

```
X <- matrix(rep(1:10, each = 10), 10, 10)
Y <- t(X)
bsxfun("*", X, Y)  # multiplication table

f <- function(x, y) x[1] * y[1]  # function not vectorized
A <- matrix(c(2, 3, 5, 7), 2, 2)
B <- matrix(c(11, 13, 17, 19), 2, 2)
arrayfun(f, A, B)</pre>
```

bulirsch-stoer

Bulirsch-Stoer Algorithm

# Description

Bulirsch-Stoer algorithm for solving Ordinary Differential Equations (ODEs) very accurately.

# Usage

```
bulirsch_stoer(f, t, y0, ..., tol = 1e-07)
midpoint(f, t0, tfinal, y0, tol = 1e-07, kmax = 25)
```

bulirsch-stoer 37

# Arguments

f	function describing the differential equation $y' = f(t, y)$ .
t	vector of x-values where the values of the ODE function will be computed; needs to be increasingly sorted.
y0	starting values as column vector.
	additional parameters to be passed to the function.
tol	relative tolerance in the Ricardson extrapolation.
t0, tfinal	start and end point of the interval.
kmax	maximal number of steps in the Richardson extrapolation.

### **Details**

The Bulirsch-Stoer algorithm is a well-known method to obtain high-accuracy solutions to ordinary differential equations with reasonable computational efforts. It exploits the midpoint method to get good accuracy in each step.

The (modified) midpoint method computes the values of the dependent variable y(t) from t0 to tfinal by a sequence of substeps, applying Richardson extrapolation in each step.

Bulirsch-Stoer and midpoint shall not be used with non-smooth functions or singularities inside the interval. The best way to get intermediate points t = (t[1], ..., t[n]) may be to call ode23 or ode23s first and use the x-values returned to start bulirsch\_stoer on.

## Value

bulirsch\_stoer returns a list with x the grid points input, and y a vector of function values at the se points.

### Note

Will be extended to become a full-blown Bulirsch-Stoer implementation.

### Author(s)

Copyright (c) 2014 Hans W Borchers

### References

J. Stoer and R. Bulirsch (2002). Introduction to Numerical Analysis. Third Edition, Texts in Applied Mathematics 12, Springer Science + Business, LCC, New York.

# See Also

ode23, ode23s

38 bvp

### **Examples**

```
## Example: y'' = -y
f1 \leftarrow function(t, y) as.matrix(c(y[2], -y[1]))
y0 <- as.matrix(c(0.0, 1.0))
tt <- linspace(0, pi, 13)</pre>
yy <- bulirsch_stoer(f1, tt, c(0.0, 1.0)) # 13 equally-spaced grid points
                                              # 1.1e-11
yy[nrow(yy), 1]
## Not run:
S \leftarrow ode23(f1, 0, pi, c(0.0, 1.0))
yy <- bulirsch_stoer(f1, S$t, c(0.0, 1.0)) # S$x 13 irregular grid points
                                              # 2.5e-11
yy[nrow(yy), 1]
S$y[nrow(S$y), 1]
                                              # -7.1e-04
## Example: y' = -200 \times y^2
                                              # y(x) = 1 / (1 + 100 x^2)
f2 \leftarrow function(t, y) -200 * t * y^2
tic(); S <- ode23(f2, 0, 1, y0); toc()
                                                     # 0.002 sec
tic(); yy <- bulirsch_stoer(f2, S$t, y0); toc() # 0.013 sec</pre>
## End(Not run)
```

bvp

Boundary Value Problems

## **Description**

Solves boundary value problems of second order differential equations.

# Usage

```
bvp(f, g, h, x, y, n = 50)
```

# **Arguments**

f, g, h	functions on the right side of the differential equation. If f, g or h is a scalar instead of a function, it is assumed to be a constant coefficient in the differential equation.
X	x[1], $x[2]$ are the interval borders where the solution shall be computed.
У	boundary conditions such that $y(x[1]) = y[1], y(x[2]) = y[2].$
n	number of intermediate grid points; default 50.

### **Details**

Solves the two-point boundary value problem given as a differential equation of second order in the form:

$$y'' = f(x)y' + g(x)y + h(x)$$

with the finite element method. The solution y(x) shall exist on the interval [a,b] with boundary conditions  $y(a) = y_a$  and  $y(b) = y_b$ .

bvp 39

### Value

Returns a list list(xs, ys) with the grid points xs and the values ys of the solution at these points, including the boundary points.

### Note

Uses a tridiagonal equation solver that may be faster then qr. solve for large values of n.

#### References

Kutz, J. N. (2005). Practical Scientific Computing. Lecture Notes 98195-2420, University of Washington, Seattle.

### See Also

newmark

```
## Solve y'' = 2*x/(1+x^2)*y' - 2/(1+x^2) * y + 1
## with y(0) = 1.25 and y(4) = -0.95 on the interval [0, 4]:
f1 \leftarrow function(x) 2*x / (1 + x^2)
f2 \leftarrow function(x) -2 / (1 + x^2)
f3 <- function(x) rep(1, length(x))
                                         # vectorized constant function 1
x < -c(0.0, 4.0)
y < -c(1.25, -0.95)
sol \leftarrow bvp(f1, f2, f3, x, y)
## Not run:
plot(sol$xs, sol$ys, ylim = c(-2, 2),
     xlab = "", ylab = "", main = "Boundary Value Problem")
# The analytic solution is
sfun \leftarrow function(x) 1.25 + 0.4860896526*x - 2.25*x^2 +
                     2*x*atan(x) - 1/2 * log(1+x^2) + 1/2 * x^2 * log(1+x^2)
xx <- linspace(0, 4)
vy <- sfun(xx)</pre>
lines(xx, yy, col="red")
grid()
## End(Not run)
## Not run:
## Solve -y'' + 0.1*y = 1 + \sin(4*pi*x)
## on [0, 1] with y(0) = y(1) = 0.
f3 \leftarrow function(x) - sin(4*pi*x) - 1
sol <- bvp(0, 0.1, f3, c(0, 1), c(0, 0), n = 40)
# The analytic solution is
fan <- function(x) cc[1]*exp(sqrt(0.1)*x) + cc[2]*exp(-sqrt(0.1)*x) +
                   1/((4*pi)^2+0.1)*sin(4*pi*x) + 10
ezplot(fan, 0, 1, col = "magenta", lty = 3)
points(sol$xs, sol$ys, type = "p", col = "blue")
grid()
## End(Not run)
```

40 cart2sph

cart2sph	Coordinate Transformations	

### Description

Transforms between cartesian, spherical, polar, and cylindrical coordinate systems in two and three dimensions.

# Usage

```
cart2sph(xyz)
sph2cart(tpr)
cart2pol(xyz)
pol2cart(prz)
```

# **Arguments**

xyz cartesian coordinates x, y, z as vector or matrix.

tpr spherical coordinates theta, phi, and r as vector or matrix.

prz polar coordinates phi, r or cylindrical coordinates phi, r, z as vector or matrix.

### **Details**

cart2sph returns spherical coordinates as (theta, phi, r), and sph2cart expects them in this sequence.

cart2pol returns polar coordinates (phi, r) if length(xyz)==2 and cylindrical coordinates (phi, r, z) else. pol2cart needs them in this sequence and length.

To go from cylindrical to cartesian coordinates, transform to cartesian coordinates first — or write your own function, see the examples.

All transformation functions are vectorized.

### Value

All functions return a (2- or 3-dimensional) vector representing a point in the requested coordinate system, or a matrix with 2 or 3 named columns where is row represents a point. The columns are named accordingly.

## Note

In Matlab these functions accept two or three variables and return two or three values. In R it did not appear appropriate to return coordinates as a list.

These functions should be vectorized in the sense that they accept will accept matrices with number of rows or columns equal to 2 or 3.

cd, pwd, what

### **Examples**

cd, pwd, what

Directory Functions (Matlab style)

# Description

Displays or changes working directory, or lists files therein.

## Usage

```
cd(dname)
pwd()
what(dname = getwd())
```

# **Arguments**

dname

(relative or absolute) directory path.

#### **Details**

pwd() displays the name of the current directory, and is the same as cd(). cd(dname) changes to directory dname and if successfull displays the directory name.

what() lists all files in a directory.

# Value

Name of the current working directory.

### See Also

```
getwd, setwd, list.files
```

42 ceil

### **Examples**

```
# cd()
# pwd()
# what()
```

ceil

Integer Functions (Matlab Style)

# Description

Functions for rounding and truncating numeric values towards near integer values.

# Usage

```
ceil(n)
Fix(n)
```

# **Arguments**

n

a numeric vector or matrix

# **Details**

ceil() is an alias for ceiling() and rounds to the smallest integer equal to or above n.

Fix() truncates values towards 0 and is an alias for trunc(). Uses ml prefix to indicate Matlab style.

The corresponding functions floor() (rounding to the largest interger equal to or smaller than n) and round() (rounding to the specified number of digits after the decimal point, default being 0) are already part of R base.

### Value

integer values

```
x <- c(-1.2, -0.8, 0, 0.5, 1.1, 2.9)

ceil(x)

Fix(x)
```

charpoly 43

charpoly

Characteristic Polynomial

## **Description**

Computes the characteristic polynomial (and the inverse of the matrix, if requested) using the Faddeew-Leverrier method.

### Usage

```
charpoly(a, info = FALSE)
```

### **Arguments**

a quadratic matrix; size should not be much larger than 100.

info logical; if true, the inverse matrix will also be reported.

### **Details**

Computes the characteristic polynomial recursively. In the last step the determinant and the inverse matrix can be determined without any extra cost (if the matrix is not singular).

### Value

Either the characteristic polynomial as numeric vector, or a list with components cp, the characteristic polynomial, det, the determinant, and inv, the inverse matrix, will be returned.

# References

Hou, S.-H. (1998). Classroom Note: A Simple Proof of the Leverrier–Faddeev Characteristic Polynomial Algorithm, SIAM Review, 40(3), pp. 706–709.

```
a <- magic(5)
A <- charpoly(a, info = TRUE)
A$cp
roots(A$cp)
A$det
zapsmall(A$inv %*% a)</pre>
```

44 chebApprox

che	ebAr	ากเ	^OX

Chebyshev Approximation

# Description

Function approximation through Chebyshev polynomials (of the first kind).

### Usage

```
chebApprox(x, fun, a, b, n)
```

# Arguments

x Numeric vector of points within interval [a, b].

fun Function to be approximated.

a, b Endpoints of the interval.

n An integer  $\geq = 0$ .

### **Details**

Return approximate y-coordinates of points at x by computing the Chebyshev approximation of degree n for fun on the interval [a, b].

# Value

A numeric vector of the same length as x.

## Note

TODO: Evaluate the Chebyshev approximative polynomial by using the Clenshaw recurrence formula. (Not yet vectorized, that's why we still use the Horner scheme.)

### References

Press, W. H., S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery (1992). Numerical Recipes in C: The Art of Scientific Computing. Second Edition, Cambridge University Press.

### See Also

polyApprox

chebCoeff 45

### **Examples**

```
# Approximate sin(x) on [-pi, pi] with a polynomial of degree 9 !
# This polynomial has to be beaten:
\# P(x) = x - \frac{1}{6}x^3 + \frac{1}{120}x^5 - \frac{1}{5040}x^7 + \frac{1}{362880}x^9
# Compare these polynomials
p1 <- rev(c(0, 1, 0, -1/6, 0, 1/120, 0, -1/5040, 0, 1/362880))
p2 <- chebCoeff(sin, -pi, pi, 9)</pre>
# Estimate the maximal distance
x <- seq(-pi, pi, length.out = 101)
ys < -sin(x)
yp <- polyval(p1, x)</pre>
yc <- chebApprox(x, sin, -pi, pi, 9)</pre>
max(abs(ys-yp))
                                         # 0.006925271
max(abs(ys-yc))
                                         # 1.151207e-05
## Not run:
# Plot the corresponding curves
plot(x, ys, type = "l", col = "gray", lwd = 5)
lines(x, yp, col = "navy")
lines(x, yc, col = "red")
grid()
## End(Not run)
```

chebCoeff

Chebyshev Polynomials

### **Description**

Chebyshev Coefficients for Chebyshev polynomials of the first kind.

## Usage

```
chebCoeff(fun, a, b, n)
```

# Arguments

```
fun function to be approximated.

a, b endpoints of the interval.

n an integer >= 0.
```

### **Details**

For a function fun on on the interval [a, b] determines the coefficients of the Chebyshev polynomials up to degree n that will approximate the function (in L2 norm).

46 chebPoly

### Value

Vector of coefficients for the Chebyshev polynomials, from low to high degrees (see the example).

#### Note

See the "Chebfun Project" <a href="http://www.maths.ox.ac.uk/chebfun/">http://www.maths.ox.ac.uk/chebfun/</a> by Nick Trefethen.

#### References

Weisstein, Eric W. "Chebyshev Polynomial of the First Kind." From MathWorld — A Wolfram Web Resource. http://mathworld.wolfram.com/ChebyshevPolynomialoftheFirstKind.html

### See Also

```
chebPoly, chebApprox
```

# **Examples**

```
## Chebyshev coefficients for x^2 + 1

n < -4

f2 < -function(x) x^2 + 1

cC < -chebCoeff(f2, -1, 1, n) # 3.0 0 0.5 0 0

cC[1] < -cC[1]/2 # correcting the absolute Chebyshev term

# i.e. 1.5*T_0 + 0.5*T_2

cP < -chebPoly(n) # summing up the polynomial coefficients

p < -cC \%*\% cP # 0 0 1 0 1
```

chebPoly

Chebyshev Polynomials

# **Description**

Chebyshev polynomials and their values.

### Usage

```
chebPoly(n, x = NULL)
```

# Arguments

```
n an integer \geq = 0.
```

x a numeric vector, possibly empty; default NULL.

### **Details**

Determines an (n+1)-ny-(n+1)-Matrix of Chebyshev polynomials up to degree n.

The coefficients of the first n Chebyshev polynomials are computed using the recursion formula. For computing any values at points the well known Horner schema is applied.

circlefit 47

### Value

If x is NULL, returns an (n+1)-by-(n+1) matrix with the coefficients of the first Chebyshev polynomials from 0 to n, one polynomial per row with coefficients from highest to lowest order.

If x is a numeric vector, returns the values of the n-th Chebyshev polynomial at the points of x.

### Note

See the "Chebfun Project" <a href="http://www.maths.ox.ac.uk/chebfun/">http://www.maths.ox.ac.uk/chebfun/</a> by Nick Trefethen.

### References

Carothers, N. L. (1998). A Short Course on Approximation Theory. Bowling Green State University, URL: http://personal.bgsu.edu/~carother/Approx.html.

# See Also

```
chebCoeff, chebApprox
```

### **Examples**

circlefit

Fitting a Circle

# **Description**

Fitting a circle from points in the plane

### Usage

```
circlefit(xp, yp)
```

48 circlefit

## Arguments

xp, yp Vectors representing the x and y coordinates of plane points

### **Details**

This routine first finds an 'algebraic' solution based on a linear fit and then calls optim with this solution as starting point.

The value to be minimized is the distance of the given points to the nearest point on the circle.

### Value

Returns x- and y-coordinates of the center and the radius as a vector of length 3.

Writes the RMS error of the distance of the original points to the circle directly onto the console.

### Note

May be worth to apply nls instead of optim.

### References

Gander, W., G. H. Golub, and R. Strebel (1994). Fitting of Circles and Ellipses — Least Squares Solutions. ETH Zürich, Technical Report 217, Institut für Wissenschaftliches Rechnen.

```
# set.seed(8421)
n <- 20
w <- 2*pi*runif(n)</pre>
xp < -cos(w) + 1 + 0.25 * (runif(n) - 0.5)
yp < -\sin(w) + 1 + 0.25 * (runif(n) - 0.5)
rslt <- circlefit(xp, yp) #=> 0.9965782 1.0009066 1.0240452
x0 <- rslt[1]; y0 <- rslt[2]; r0 <- rslt[3]</pre>
## Not run:
plot(c(-0.2, 2.2), c(-0.2, 2.2), type="n", asp=1)
abline(h=0, col="gray"); abline(v=0, col="gray")
points(xp, yp, col="darkred")
w < - seq(0, 2*pi, len=100)
xx <- r0 * cos(w) + x0
yy < - r0 * sin(w) + y0
lines(xx, yy, col="blue")
## End(Not run)
```

clear, who(s), ver

```
clear, who(s), ver
```

Clear function (Matlab style)

# Description

List or remove items from workspace, or display system information.

# Usage

```
clear(lst)
ver()
who()
whos()
```

# Arguments

lst

Character vector of names of variables in the global environment.

# **Details**

Remove these or all items from the workspace, i.e. the global environment, and freeing up system memory.

```
who() lists all items on the workspace.
```

whos() lists all items and their class and size.

ver() displays version and license information for R and all the loaded packages.

# Value

Invisibly NULL.

### See Also

```
ls, rm, sessionInfo
```

```
# clear() # DON'T
# who()
# whos()
# ver()
```

50 clenshaw\_curtis

clenshaw\_curtis

Clenshaw-Curtis Quadrature Formula

# **Description**

Clenshaw-Curtis Quadrature Formula

# Usage

```
clenshaw_curtis(f, a = -1, b = 1, n = 1024, ...)
```

# **Arguments**

f function, the integrand, without singularities.
 a, b lower and upper limit of the integral; must be finite.
 n Number of Chebyshev nodes to account for.

... Additional parameters to be passed to the function

# **Details**

Clenshaw-Curtis quadrature is based on sampling the integrand on Chebyshev points, an operation that can be implemented using the Fast Fourier Transform.

## Value

Numerical scalar, the value of the integral.

### References

```
Trefethen, L. N. (2008). Is Gauss Quadrature Better Than Clenshaw-Curtis?. http://www.comlab.ox.ac.uk/nick.trefethen/CC.pdf.
```

#### See Also

```
gaussLegendre, gauss_kronrod
```

```
## Quadrature with Chebyshev nodes and weights f <- \text{ function}(x) \sin(x + \cos(10 * \exp(x))/3) ## Not run: ezplot(f, -1, 1, fill = TRUE) cc <- \text{ clenshaw\_curtis}(f, n = 64) \text{ #=> } 0.0325036517151 \text{ , true error > } 1.3e-10
```

combs 51

combs

Generate Combinations

# Description

Generates all combinations of length m of a vector a.

# Usage

```
combs(a, m)
```

# **Arguments**

```
a numeric vector of some length n m integer with 0 \le m \le n
```

# **Details**

combs generates combinations of length n of the elements of the vector a.

# Value

matrix representing combinations of the elements of a

# See Also

```
perms, randcomb
```

# **Examples**

```
combs(seq(2, 10, by=2), m = 3)
```

compan

Companion Matrix

# Description

Computes the companion matrix of a vector.

# Usage

```
compan(p)
```

# **Arguments**

р

vector representing a polynomial

52 complexstep

### **Details**

Computes the companion matrix corresponding to the vector p with -p[2:length(p)]/p[1] as first row.

The eigenvalues of this matrix are the roots of the polynomial.

# Value

A square matrix of length(p)-1 rows and columns

### See Also

roots

# **Examples**

```
p <- c(1, 0, -7, 6)
compan(p)
# 0 7 -6
# 1 0 0
# 0 1 0
```

complexstep

Complex Step Derivatives

# Description

Complex step derivatives of real-valued functions, including gradients, Jacobians, and Hessians.

# Usage

```
complexstep(f, x0, h = 1e-20, ...)
grad_csd(f, x0, h = 1e-20, ...)
jacobian_csd(f, x0, h = 1e-20, ...)
hessian_csd(f, x0, h = 1e-20, ...)
laplacian_csd(f, x0, h = 1e-20, ...)
```

# **Arguments**

f	Function that is to be differentiated.
x0	Point at which to differentiate the function.
h	Step size to be applied; shall be very small.
	Additional variables to be passed to f.

complexstep 53

### **Details**

Complex step derivation is a fast and highly exact way of numerically differentiating a function. If the following conditions are satisfied, there will be no loss of accuracy between computing a function value and computing the derivative at a certain point.

- f must have an analytical (i.e., complex differentiable) continuation into an open neighborhood of x0.
- x0 and f(x0) must be real.
- h is real and *very* small: 0 < h << 1.

complexstep handles differentiation of univariate functions, while grad\_csd and jacobian\_csd compute gradients and Jacobians by applying the complex step approach iteratively. Please understand that these functions are not vectorized, but complexstep is.

As complex step cannot be applied twice (the first derivative does not fullfil the conditions), hessian\_csd works differently. For the first derivation, complex step is used, to the one time derived function Richardson's method is applied. The same applies to lapalacian\_csd.

#### Value

```
complexstep(f, x0) returns the derivative f'(x_0) of f at x_0. The function is vectorized in x0.
```

#### Note

This surprising approach can be easily deduced from the complex-analytic Taylor formula.

### Author(s)

HwB < hwborchers@googlemail.com>

### References

Martins, J. R. R. A., P. Sturdza, and J. J. Alonso (2003). The Complex-step Derivative Approximation. ACM Transactions on Mathematical Software, Vol. 29, No. 3, pp. 245–262.

#### See Also

numderiv

```
## Example from Martins et al.
f <- function(x) exp(x)/sqrt(sin(x)^3 + cos(x)^3)  # derivative at x0 = 1.5
# central diff formula  # 4.05342789402801, error 1e-10
# numDeriv::grad(f, 1.5)  # 4.05342789388197, error 1e-12 Richardson
# pracma::numderiv  # 4.05342789389868, error 5e-14 Richardson
complexstep(f, 1.5)  # 4.05342789389862, error 1e-15
# Symbolic calculation:  # 4.05342789389862
jacobian_csd(f, 1.5)</pre>
```

54 cond

```
f1 <- function(x) sum(sin(x))</pre>
grad_csd(f1, rep(2*pi, 3))
## [1] 1 1 1
laplacian_csd(f1, rep(pi/2, 3))
## [1] -3
f2 \leftarrow function(x) c(sin(x[1]) * exp(-x[2]))
hessian_csd(f2, c(0.1, 0.5, 0.9))
                            [,2][,3]
                [,1]
## [1,] -0.06055203 -0.60350053
                                     0
## [2,] -0.60350053 0.06055203
                                     0
## [3,] 0.00000000 0.00000000
                                     0
f3 <- function(u) {
    x \leftarrow u[1]; y \leftarrow u[2]; z \leftarrow u[3]
   matrix(c(exp(x^+y^2), sin(x+y), sin(x)*cos(y), x^2 - y^2), 2, 2)
jacobian_csd(f3, c(1,1,1))
              [,1]
                          [,2][,3]
## [1,] 2.7182818 0.0000000
## [2,] -0.4161468 -0.4161468
                                   0
## [3,] 0.2919266 -0.7080734
                                   0
## [4,] 2.0000000 -2.0000000
```

cond

Matrix Condition

# **Description**

Condition number of a matrix.

# Usage

```
cond(M, p = 2)
```

# **Arguments**

M Numeric matrix; vectors will be considered as column vectors.

p Indicates the p-norm. At the moment, norms other than p=2 are not implemented.

# **Details**

The condition number of a matrix measures the sensitivity of the solution of a system of linear equations to small errors in the data. Values of cond(M) and cond(M, p) near 1 are indications of a well-conditioned matrix.

conv 55

### Value

cond(M) returns the 2-norm condition number, the ratio of the largest singular value of M to the smallest.

```
c = cond(M, p) returns the matrix condition number in p-norm:

norm(X,p) * norm(inv(X),p).

(Not yet implemented.)
```

# Note

Not feasible for large or sparse matrices as svd(M) needs to be computed. The Matlab/Octave function condest for condition estimation has not been implemented.

### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Philadelphia.

# See Also

```
normest, svd
```

# **Examples**

```
cond(hilb(8))
```

conv

Polynomial Convolution

# **Description**

Convolution and polynomial multiplication.

# Usage

```
conv(x, y)
```

# Arguments

х, у

real or complex vectors.

### **Details**

r = conv(p,q) convolves vectors p and q. Algebraically, convolution is the same operation as multiplying the polynomials whose coefficients are the elements of p and q.

# Value

Another vector.

56 cot,csc,sec, etc.

# Note

conv utilizes fast Fourier transformation.

### See Also

```
deconv, polyadd
```

# **Examples**

```
conv(c(1, 1, 1), 1)
conv(c(1, 1, 1), c(0, 0, 1))
conv(c(-0.5, 1, -1), c(0.5, 0, 1))
```

cot,csc,sec, etc.

More Trigonometric Functions

# Description

More trigonometric functions not available in R.

# Usage

cot(z)
csc(z)
sec(z)
acot(z)
acsc(z)

acsc(z)

# Arguments

z numeric or complex scalar or vector.

# **Details**

The usual trigonometric cotangens, cosecans, and secans functions and their inverses, computed through the other well known – in R – sine, cosine, and tangens functions.

## Value

Result vector of numeric or complex values.

# Note

These function names are available in Matlab, that is the reason they have been added to the 'pracma' package.

cotes 57

### See Also

Trigonometric and hyperbolic functions in R.

### **Examples**

```
cot(1+1i) # 0.2176 - 0.8680i

csc(1+1i) # 0.6215 - 0.3039i

sec(1+1i) # 0.4983 + 0.5911i

acot(1+1i) # 0.5536 - 0.4024i

acsc(1+1i) # 0.4523 - 0.5306i

asec(1+1i) # 1.1185 + 0.5306i
```

cotes

Newton-Cotes Formulas

# **Description**

Closed composite Newton-Cotes formulas of degree 2 to 8.

## Usage

```
cotes(f, a, b, n, nodes, ...)
```

# **Arguments**

f	the integrand as function of two variables.
a, b	lower and upper limit of the integral.
n	number of subintervals (grid points).
nodes	number of nodes in the Newton-Cotes formula.
	additional parameters to be passed to the function.

# **Details**

2 to 8 point closed and summed Newton-Cotes numerical integration formulas.

These formulas are called 'closed' as they include the endpoints. They are called 'composite' insofar as they are combined with a Lagrange interpolation over subintervals.

## Value

The integral as a scalar.

# Note

It is generally recommended not to apply Newton-Cotes formula of degrees higher than 6, instead increase the number n of subintervals used.

58 coth,csch,sech, etc.

### Author(s)

Standard Newton-Cotes formulas can be found in every textbook. Copyright (c) 2005 Greg von Winckel of nicely vectorized Matlab code, available from MatlabCentral, for 2 to 11 grid points. R version by Hans W Borchers, with permission.

#### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

```
simpadpt, trapz
```

## **Examples**

```
cotes(sin, 0, pi/2, 20, 2)  # 0.999485905248533
cotes(sin, 0, pi/2, 20, 3)  # 1.000000211546591
cotes(sin, 0, pi/2, 20, 4)  # 1.000000391824184
cotes(sin, 0, pi/2, 20, 5)  # 0.99999999501637
cotes(sin, 0, pi/2, 20, 6)  # 0.99999998927507
cotes(sin, 0, pi/2, 20, 7)  # 1.00000000000363 odd degree is better
cotes(sin, 0, pi/2, 20, 8)  # 1.000000000002231
```

```
coth, csch, sech, etc. More Hyperbolic Functions
```

### **Description**

More hyperbolic functions not available in R.

# Usage

```
coth(z)
csch(z)
sech(z)
acoth(z)
acsch(z)
asech(z)
```

# Arguments

z numeric or complex scalar or vector.

### **Details**

The usual hyperbolic cotangens, cosecans, and secans functions and their inverses, computed through the other well known – in R – hyperbolic sine, cosine, and tangens functions.

cranknic 59

# Value

Result vector of numeric or complex values.

### Note

These function names are available in Matlab, that is the reason they have been added to the 'pracma' package.

### See Also

Trigonometric and hyperbolic functions in R.

### **Examples**

```
coth(1+1i) # 0.8680 - 0.2176i

csch(1+1i) # 0.3039 - 0.6215i

sech(1+1i) # 0.4983 - 0.5911i

acoth(1+1i) # 0.4024 - 0.5536i

acsch(1+1i) # 0.5306 - 0.4523i

asech(1+1i) # 0.5306 - 1.1185i
```

cranknic

Crank-Nicolson Method

# **Description**

The Crank-Nicolson method for solving ordinary differential equations is a combination of the generic steps of the forward and backward Euler methods.

# Usage

```
cranknic(f, t0, t1, y0, ..., N = 100)
```

### **Arguments**

f	function in the differential equation $y' = f(x, y)$ ; defined as a function $R \times R^m \to R^m$ , where m is the number of equations.
t0, t1	start and end points of the interval.
y0	starting values as row or column vector; for $m$ equations y0 needs to be a vector of length $\mathbf{m}$ .
N	number of steps.
	Additional parameters to be passed to the function.

### **Details**

Adding together forward and backword Euler method in the cranknic method is by finding the root of the function merging these two formulas.

No attempt is made to catch any errors in the root finding functions.

60 cranknic

### Value

List with components t for grid (or 'time') points between t0 and t1, and y an n-by-m matrix with solution variables in columns, i.e. each row contains one time stamp.

### Note

This is for demonstration purposes only; for real problems or applications please use ode23 or rkf54.

#### References

Quarteroni, A., and F. Saleri (2006). Scientific Computing With MATLAB and Octave. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

```
ode23, newmark
```

```
## Newton's example
f \leftarrow function(x, y) 1 - 3*x + y + x^2 + x*y
sol100 <- cranknic(f, 0, 1, 0, N = 100)
sol1000 \leftarrow cranknic(f, 0, 1, 0, N = 1000)
## Not run:
# Euler's forward approach
feuler <- function(f, t0, t1, y0, n) {</pre>
    h \leftarrow (t1 - t0)/n; x \leftarrow seq(t0, t1, by = h)
    y <- numeric(n+1); y[1] <- y0</pre>
    for (i in 1:n) y[i+1] \leftarrow y[i] + h * f(x[i], y[i])
    return(list(x = x, y = y))
solode <- ode23(f, 0, 1, 0)
soleul <- feuler(f, 0, 1, 0, 100)
plot(soleul$x, soleul$y, type = "1", col = "blue",
     xlab = "", ylab = "", main = "Newton's example")
lines(solode$t, solode$y, col = "gray", lwd = 3)
lines(sol100$t, sol100$y, col = "red")
lines(sol1000$t, sol1000$y, col = "green")
grid()
## System of differential equations
# "Herr und Hund"
fhh <- function(x, y) {</pre>
    y1 \leftarrow y[1]; y2 \leftarrow y[2]
    s \leftarrow sqrt(y1^2 + y2^2)
    dy1 < -0.5 - 0.5*y1/s
    dy2 < -0.5*y2/s
```

cross 61

cross

Vector Cross Product

# **Description**

Vector or cross product

# Usage

```
cross(x, y)
```

# **Arguments**

x numeric vector or matrix y numeric vector or matrix

### **Details**

Computes the cross (or: vector) product of vectors in 3 dimensions. In case of matrices it takes the first dimension of length 3 and computes the cross product between corresponding columns or rows.

The more general cross product of n-1 vectors in n-dimensional space is realized as crossn.

### Value

3-dim. vector if x and < are vectors, a matrix of 3-dim. vectors if x and y are matrices themselves.

### See Also

```
dot, crossn
```

```
cross(c(1, 2, 3), c(4, 5, 6)) # -3 6 -3
```

62 crossn

crossn

n-dimensional Vector Cross Product

# **Description**

Vector cross product of n-1 vectors in n-dimensional space

### Usage

```
crossn(A)
```

# **Arguments**

Α

```
matrix of size (n-1) \times n where n \ge 2.
```

### **Details**

The rows of the matrix A are taken as(n-1) vectors in n-dimensional space. The cross product generates a vector in this space that is orthogonal to all these rows in A and its length is the volume of the geometric hypercube spanned by the vectors.

## Value

```
a vector of length n
```

### Note

```
The 'scalar triple product' in \mathbb{R}^3 can be defined as spatproduct <- function(a, b, c) dot(a, crossn(b, c)) It represents the volume of the parallelepiped spanned by the three vectors.
```

### See Also

```
cross, dot
```

```
A <- matrix(c(1,0,0,0,1,0), nrow=2, ncol=3, byrow=TRUE) crossn(A) #=> 0 0 1  x <- c(1.0, 0.0, 0.0) \\ y <- c(1.0, 0.5, 0.0) \\ z <- c(0.0, 0.0, 1.0) \\ identical(dot(x, crossn(rbind(y, z))), det(rbind(x, y, z)))
```

cubicspline 63

# Description

Computes the natural interpolation cubic spline.

# Usage

```
cubicspline(x, y, xi = NULL, endp2nd = FALSE, der = c(0, 0))
```

# **Arguments**

x, y	x- and y-coordinates of points to be interpolated.
xi	x-coordinates of points at which the interpolation is to be performed.
endp2nd	logical; if true, the derivatives at the endpoints are prescribed by der.
der	a two-components vector prescribing derivatives at endpoints.

### **Details**

cubicspline computes the values at xi of the natural interpolating cubic spline that interpolate the values y at the nodes x. The derivatives at the endpoints can be prescribed.

# Value

Returns either the interpolated values at the points xi or, if is.null(xi), the piecewise polynomial that represents the spline.

# Note

From the piecewise polynomial returned one can easily generate the spline function, see the examples.

# References

Quarteroni, Q., and F. Saleri (2006). Scientific Computing with Matlab and Octave. Springer-Verlag Berlin Heidelberg.

# See Also

spline

64 curvefit

### **Examples**

```
## Example: Average temperatures at different latitudes
x < - seq(-55, 65, by = 10)
y < -c(-3.25, -3.37, -3.35, -3.20, -3.12, -3.02, -3.02,
       -3.07, -3.17, -3.32, -3.30, -3.22, -3.10)
xs < - seq(-60, 70, by = 1)
# Generate a function for this
pp <- cubicspline(x, y)</pre>
ppfun <- function(xs) ppval(pp, xs)</pre>
## Not run:
# Plot with and without endpoint correction
plot(x, y, col = "darkblue",
           xlim = c(-60, 70), ylim = c(-3.5, -2.8),
           xlab = "Latitude", ylab = "Temp. Difference",
           main = "Earth Temperatures per Latitude")
lines(spline(x, y), col = "darkgray")
grid()
ys <- cubicspline(x, y, xs, endp2nd = TRUE)</pre>
                                                  # der = 0 at endpoints
lines(xs, ys, col = "red")
ys <- cubicspline(x, y, xs)</pre>
                                                  # no endpoint condition
lines(xs, ys, col = "darkred")
## End(Not run)
```

curvefit

Parametric Curve Fit

### **Description**

Polynomial fitting of parametrized points on 2D curves, also requiring to meet some points exactly.

### Usage

```
curvefit(u, x, y, n, U = NULL, V = NULL)
```

# Arguments

u	the parameter vector.
x, y	x-, y-coordinates for each parameter value.
n	order of the polynomials, the same in x- and y-direction.
U	parameter values where points will be fixed.
V	matrix with two columns and lemgth(U) rows; first column contains the x-, the second the y-values of those points kept fixed.

curvefit 65

### **Details**

This function will attempt to fit two polynomials to parametrized curve points using the linear least squares approach with linear equality constraints in lsqlin. The requirement to meet exactly some fixed points is interpreted as a linear equality constraint.

### Value

Returns a list with 4 components, xp and yp coordinates of the fitted points, and px and py the coefficients of the fitting polynomials in x- and y-direction.

#### Note

In the same manner, derivatives/directions could be prescribed at certain points.

### See Also

```
circlefit, lsqlin
```

```
## Approximating half circle arc with small perturbations
N <- 50
u <- linspace(0, pi, N)</pre>
x < -\cos(u) + 0.05 * randn(1, N)
y <- \sin(u) + 0.05 * randn(1, N)
n <- 8
cfit1 <- curvefit(u, x, y, n)
## Not run:
plot(x, y, col = "darkgray", pch = 19, asp = 1)
xp <- cfit1$xp; yp <- cfit1$yp
lines(xp, yp, col="blue")
grid()
## End(Not run)
## Fix the end points at t = 0 and t = pi
U <- c(0, pi)
V \leftarrow matrix(c(1, 0, -1, 0), 2, 2, byrow = TRUE)
cfit2 <- curvefit(u, x, y, n, U, V)
## Not run:
xp <- cfit2$xp; yp <- cfit2$yp
lines(xp, yp, col="red")
## End(Not run)
## Not run:
## Archimedian spiral
u <- linspace(0, 3*pi, 50)
a <- 1.0
x <- as.matrix(a*u*cos(u))</pre>
y <- as.matrix(a*u*sin(u))</pre>
plot(x, y, type = "p", pch = 19, col = "darkgray", asp = 1)
```

66 cutpoints

```
lines(x, y, col = "darkgray", lwd = 3)
cfit <- curvefit(u, x, y, n)
px <- c(cfit$px); py <- c(cfit$py)
v <- linspace(0, 3*pi, 200)
xs <- polyval(px, v)
ys <- polyval(py, v)
lines(xs, ys, col = "navy")
grid()
## End(Not run)</pre>
```

cutpoints

Find Cutting Points

# **Description**

Finds cutting points for vector s of real numbers.

### **Usage**

```
cutpoints(x, nmax = 8, quant = 0.95)
```

# **Arguments**

x vector of real values.

nmax the maximum number of cutting points to choose

quantile of the gaps to consider for cuts.

#### **Details**

Finds cutting points for vector s of real numbers, based on the gaps in the values of the vector. The number of cutting points is derived from a quantile of gaps in the values. The user can set a lower limit for this number of gaps.

### Value

Returns a list with components cutp, the cutting points selected, and cutd, the gap between values of x at this cutting point.

### Note

Automatically finding cutting points is often requested in Data Mining. If a target attribute is available, Quinlan's C5.0 does a very good job here. Unfortunately, the 'C5.0' package (of the R-Forge project "Rulebased Models") is quite cumbersome to use.

### References

Witten, I. H., and E. Frank (2005). Data Mining: Practical Machine Learning Tools and Techniques. Morgan Kaufmann Publishers, San Francisco.

dblquad 67

## See Also

cut

```
N \leftarrow 100; x \leftarrow sort(runif(N))
cp \leftarrow cutpoints(x, 6, 0.9)
n <- length(cp$cutp)</pre>
# Print out
nocp \leftarrow rle(findInterval(x, c(-Inf, cp$cutp, Inf)))$lengths
cbind(c(-Inf, cp$cutp), c(cp$cutp, Inf), nocp)
# Define a factor from the cutting points
fx \leftarrow cut(x, breaks = c(-Inf, cp$cutp, Inf))
## Not run:
# Plot points and cutting points
plot(x, rep(0, N), col="gray", ann = FALSE)
points(cp$cutp, rep(0, n), pch="|", col=2)
# Compare with k-means clustering
km <- kmeans(x, n)
points(x, rep(0, N), col = km$cluster, pch = "+")
## A 2-dimensional example
x <- y <- c()
for (i in 1:9) {
  for (j in 1:9) {
    x \leftarrow c(x, i + rnorm(20, 0, 0.2))
    y \leftarrow c(y, j + rnorm(20, 0, 0.2))
}
cpx \leftarrow cutpoints(x, 8, 0)
cpy <- cutpoints(y, 8, 0)</pre>
plot(x, y, pch = 18, col=rgb(0.5, 0.5, 0.5), axes=FALSE, ann=FALSE)
for (xi in cpx$cutp) abline(v=xi, col=2, lty=2)
for (yi in cpy$cutp) abline(h=yi, col=2, lty=2)
km <- kmeans(cbind(x, y), 81)
points(x, y, col=km$cluster)
## End(Not run)
```

68 dblquad

## **Description**

Numerically evaluate double integral over rectangle.

# Usage

### **Arguments**

f	function of two variables, the integrand.
xa, xb	left and right endpoint for first variable.
ya, yb	left and right endpoint for second variable.
za, zb	left and right endpoint for third variable.
dim	which variable to integrate first.
subdivs	number of subdivisions to use.
tol	relative tolerance to use in integrate.
	additional parameters to be passed to the integrand.

## **Details**

Function dblquad applies the internal single variable integration function integrate two times, once for each variable.

Function triplequad reduces the problem to dblquad by first integrating over the innermost variable.

### Value

Numerical scalar, the value of the integral.

### See Also

```
integrate, quad2d, simpson2d
```

```
f1 <- function(x, y) x^2 + y^2

dblquad(f1, -1, 1, -1, 1) # 2.666666667 , i.e. 8/3 . err = 0

f2 <- function(x, y) y*sin(x)+x*cos(y)

dblquad(f2, pi, 2*pi, 0, pi) # -9.869604401 , i.e. -pi^2, err = 0

# f3 <- function(x, y) sqrt((1 - (x^2 + y^2)) * (x^2 + y^2 <= 1))

f3 <- function(x, y) sqrt(pmax(0, 1 - (x^2 + y^2)))
```

deconv 69

```
dblquad(f3, -1, 1, -1, 1)  # 2.094395124 , i.e. 2/3*pi , err = 2e-8 f4 <- function(x, y, z) y*sin(x)+z*cos(x) triplequad(f4, 0,pi, 0,1, -1,1) # - 2.0 => -2.220446e-16
```

deconv

Deconvolution

# **Description**

Deconvolution and polynomial division.

## Usage

```
deconv(b, a)
```

# Arguments

b, a

real or complex vectors.

### **Details**

deconv(b,a) deconvolves vector a out of vector b. The quotient is returned in vector q and the remainder in vector r such that b = conv(a,q)+r.

If b and a are vectors of polynomial coefficients, convolving them is equivalent to multiplying the two polynomials, and deconvolution is polynomial division.

# Value

List with elements named q and r.

# Note

TODO: Base deconv on some filter1d function.

### See Also

```
conv, polymul
```

```
b <- c(10, 40, 100, 160, 170, 120)
a <- c(1, 2, 3, 4)
p <- deconv(b, a)
p$q  #=> 10 20 30
p$r  #=> 0 0 0
```

70 deeve

deeve

Event Detection in ODE solution

# **Description**

Detect events in solutions of a differential equation.

### Usage

```
deeve(x, y, yv = 0, idx = NULL)
```

# **Arguments**

Х	vector of (time) points at which the differential equation has been solved.
у	values of the function(s) that have been computed for the given (time) points.
yv	point or numeric vector at which the solution is wanted.
idx	index of functions whose vales shall be returned.

### **Details**

Determines when (in x coordinates) the idx-th solution function will take on the value yv. The interpolation is linear for the moment. For points outside the x interval NA is returned.

# Value

A (time) point x0 at which the event happens.

# Note

The interpolation is linear only for the moment.

# See Also

deval

```
## Damped pendulum: y'' = -0.3 y' - sin(y)
# y1 = y, y2 = y': y1' = y2, y2' = -0.3*y2 - sin(y1)
f <- function(t, y) {
    dy1 <- y[2]
    dy2 <- -0.3*y[2] - sin(y[1])
    return(c(dy1, dy2))
}
sol <- rk4sys(f, 0, 10, c(pi/2, 0), 100)
deeve(sol$x, sol$y[,1])  # y1 = 0 : elongation in [sec]
# [1] 2.073507 5.414753 8.650250
# matplot(sol$x, sol$y); grid()</pre>
```

deg2rad 71

deg2rad

Degrees to Radians

# Description

Transforms between angles in degrees and radians.

### Usage

```
deg2rad(deg)
rad2deg(rad)
```

# **Arguments**

```
deg (array of) angles in degrees.
rad (array of) angles in radians.
```

### **Details**

This is a simple calculation back and forth. Note that angles greater than 360 degrees are allowed and will be returned. This may appear incorrect but follows a corresponding discussion on Matlab Central.

### Value

The angle in degrees or radians.

# **Examples**

```
deg2rad(c(0, 10, 20, 30, 40, 50, 60, 70, 80, 90))
rad2deg(seq(-pi/2, pi/2, length = 19))
```

detrend

Remove Linear Trends

# **Description**

Removes the mean value or (piecewise) linear trend from a vector or from each column of a matrix.

# Usage

```
detrend(x, tt = 'linear', bp = c())
```

72 deval

# **Arguments**

X	vector or matrix, columns considered as the time series.
tt	trend type, 'constant' or 'linear', default is 'linear'.
bp	break points, indices between 1 and nrow(x).

# **Details**

detrend computes the least-squares fit of a straight line (or composite line for piecewise linear trends) to the data and subtracts the resulting function from the data.

To obtain the equation of the straight-line fit, use polyfit.

### Value

removes the mean or (piecewise) linear trend from x and returns it in y=detrend(x), that is x-y is the linear trend.

### Note

Detrending is often used for FFT processing.

### See Also

```
polyfit
```

# **Examples**

```
t <- 1:9
x <- c(0, 2, 0, 4, 4, 4, 0, 2, 0)
x - detrend(x, 'constant')
x - detrend(x, 'linear')

y <- detrend(x, 'linear', 5)
## Not run:
plot(t, x, col="blue")
lines(t, x - y, col="red")
grid()
## End(Not run)</pre>
```

deval

**Evaluate ODE Solution** 

## **Description**

Evaluate solution of a differential equation solver.

# Usage

```
deval(x, y, xp, idx = NULL)
```

Diag 73

## **Arguments**

X	vector of (time) points at which the differential equation has been solved.
у	values of the function(s) that have been computed for the given (time) points.
xp	point or numeric vector at which the solution is wanted; must be sorted.
idx	index of functions whose vales shall be returned.

## **Details**

Determines where the points xp lie within the vector x and interpolates linearly.

#### Value

```
An length(xp)-by-length(idx) matrix of values at points xp.
```

### Note

The interpolation is linear only for the moment.

## See Also

deeve

## **Examples**

```
## Free fall: v' = -g - cw abs(v)^1.1, cw = 1.6 drag coefficien
f <- function(t, y) -9.81 + 1.6*abs(y)^1.1
sol <- rk4(f, 0, 10, 0, 100)
# speed after 0.5, 1, 1.5, 2 seconds
cbind(c(0.5,1,1.5,2), -deval(sol$x, sol$y, c(0.5, 1, 1.5, 2)))
# 0.5 3.272267 m/s
# 1.0 4.507677
# 1.5 4.953259
# 2.0 5.112068
# plot(sol$x, -sol$y, type="1", col="blue"); grid()</pre>
```

Diag

Matrix Diagonal

## **Description**

Generate diagonal matrices or return diagonal of a matrix

## Usage

```
Diag(x, k = 0)
```

74 direct1d

## **Arguments**

- x vector or matrix
- k integer indicating a secondary diagonal

#### **Details**

If x is a vector, Diag(x, k) generates a matrix with x as the (k-th secondary) diagonal.

If x is a matrix, Diag(x, k) returns the (k-th secondary) diagonal of x.

The k-th secondary diagonal is above the main diagonal for k > 0 and below the main diagonal for k < 0.

## Value

matrix or vector

### Note

In Matlab/Octave this function is called diag() and has a different signature than the corresponding function in R.

#### See Also

```
diag, Trace
```

# **Examples**

```
Diag(matrix(1:12,3,4), 1)
Diag(matrix(1:12,3,4), -1)
Diag(c(1,5,9), 1)
Diag(c(1,5,9), -1)
```

direct1d

Univariate Global Optimization

# Description

Implementation of the DIRECT global optimization algorithm in the one-dimensional case.

## Usage

```
direct1d(f, a, b, maxiter = 20, ...)
```

direct1d 75

## **Arguments**

f	function to be minimized.
a, b	end points of the interval, a <b.< td=""></b.<>
maxiter	maximum number of iterations.
	further parameters to be passed to the function.

### **Details**

The DIRECT algorithm for the one-dimensional case is directly derived from Shubert's algorithm. Instead of computing the function at the endpoints of the interval, it is computed at the midpoint. Intervals ar split in three parts, sparing one function evaluation.

### Value

List with components xmin and fmin, the minimum found so far and its function value.

#### Note

The subroutine for finding the set of optimal subintervals is slow and has to be intelligently refitted.

## Author(s)

HwB email: <a href="mailto:</a> <a href="mailto:hwborchers@googlemail.com">hwborchers@googlemail.com</a>

#### References

Jones, D. R., C. D. Perttunen, and B. E. Stuckman (1993). Lipschitzian Optimization Without the Lipschitz Constant. Journal of Optimization Theory and Application, Vol. 79. No. 1, pp. 157ff.

Finkel, D., and C. Kelley (2006). Additive Scaling and the DIRECT Algorithm. Journal of Global Optimization, Vol. 36, No. 4, pp. 597–608.

### See Also

```
findmins, dfoptim::direct
```

```
f <- function(x) sin(10*pi*x) + 0.5*(x-0.5)^2
a <- 0; b <- 1
direct1d(f, 0, 1, maxiter = 20)
# $xmin: 0.5499493794 (error: 3.5e-6)
# $fmin: -0.9987512652
## Not run:
ezplot(f, a, b, 1000)
## End(Not run)</pre>
```

76 distmat

disp,beep

Utility functions (Matlab style)

# Description

Display text or array, or produce beep sound.

# Usage

```
disp(...)
beep()
```

### **Arguments**

... any R object that can be printed.

### **Details**

Display text or array, or produces the computer's default beep sound using 'cat' with closing newline.

### Value

beep() returns NULL invisibly, disp() displays with newline.

# **Examples**

```
disp("Some text, and numbers:", pi, exp(1))
# beep()
```

distmat

Distance Matrix

# Description

Computes the Euclidean distance between rows of two matrices.

## Usage

```
distmat(X, Y)
pdist(X)
pdist2(X, Y)
```

## Arguments

```
X matrix of some size m x k; vector will be taken as row matrix.
Y matrix of some size n x k; vector will be taken as row matrix.
```

distmat 77

### **Details**

Computes Euclidean distance between two vectors A and B as:

```
||A-B|| = sqrt ( ||A||^2 + ||B||^2 - 2*A.B ) and vectorizes to rows of two matrices (or vectors). pdist2 is an alias for distmat, while pdist(X) is the same as distmat(X, X).
```

### Value

matrix of size  $m \times n$  if x is of size  $m \times k$  and y is of size  $n \times k$ .

#### Note

```
If a is m x r and b is n x r then apply(outer(a,t(b),"-"),c(1,4),function(x)sqrt(sum(diag(x*x))))
```

is the m x n matrix of distances between the m rows of a and n rows of b.

This can be modified as necessary, if one wants to apply distances other than the euclidean.

BUT: The code shown here is 10-100 times faster, utilizing the similarity between Euclidean distance and matrix operations.

#### References

Copyright (c) 1999 Roland Bunschoten for a Matlab version on MatlabCentral under the name distance.m. Translated to R by Hans W Borchers.

## See Also

dist

```
A <- c(0.0, 0.0)
B <- matrix(c(
          0,0, 1,0, 0,1, 1,1), nrow=4, ncol = 2, byrow = TRUE)
distmat(A, B) #=> 0 1 1 sqrt(2)

X <- matrix(rep(0.5, 5), nrow=1, ncol=5)
Y <- matrix(runif(50), nrow=10, ncol=5)
distmat(X, Y)</pre>
```

78 eig

dot

Scalar Product

# Description

'dot' or 'scalar' product of vectors or pairwise columns of matrices.

## Usage

```
dot(x, y)
```

### **Arguments**

x numeric vector or matrix y numeric vector or matrix

#### **Details**

Returns the 'dot' or 'scalar' product of vectors or columns of matrices. Two vectors must be of same length, two matrices must be of the same size. If x and y are column or row vectors, their dot product will be computed as if they were simple vectors.

## Value

A scalar or vector of length the number of columns of x and y.

### See Also

cross

# **Examples**

```
dot(1:5, 1:5) #=> 55
# Length of space diagonal in 3-dim- cube:
sqrt(dot(c(1,1,1), c(1,1,1))) #=> 1.732051
```

eig

Eigenvalue Function (Matlab Style)

# Description

Eigenvalues of a matrix

## Usage

eig(a)

eigjacobi 79

### **Arguments**

а

real or complex square matrix

#### **Details**

Computes the eigenvalues of a square matrix of real or complex numbers, using the R routine eigen without computing the eigenvectors.

#### Value

Vector of eigenvalues

#### See Also

compan

## **Examples**

```
\begin{array}{lll} \text{eig}(\text{matrix}(c(1,-1,-1,1),\ 2,\ 2)) & \ \#=>\ 2\ 0 \\ \text{eig}(\text{matrix}(c(1,1,-1,1),\ 2,\ 2)) & \ \#\ \text{complex\ values} \\ \text{eig}(\text{matrix}(c(0,1i,-1i,0),\ 2,\ 2)) & \ \#\ \text{real\ values} \end{array}
```

eigjacobi

Jacobi Eigenvalue Method

## **Description**

Jacobi's iteration method for eigenvalues and eigenvectors.

# Usage

```
eigjacobi(A, tol = .Machine$double.eps^(2/3))
```

# Arguments

A a real symmetric matrix.

tol requested tolerance.

#### **Details**

The Jacobi eigenvalue method repeatedly performs (Givens) transformations until the matrix becomes almost diagonal.

### Value

Returns a list with components V, a matrix containing the eigenvectors as columns, and D a vector of the eigenvalues.

80 einsteinF

### Note

This R implementation works well up to 50x50-matrices.

#### References

Mathews, J. H., and K. D. Fink (2004). Numerical Methods Using Matlab. Fourth edition, Pearson education, Inc., New Jersey.

### See Also

eig

## **Examples**

```
A <- matrix(c( 1.06, -0.73, 0.77, -0.67, -0.73, 2.64, 1.04, 0.72, 0.77, 1.04, 3.93, -2.14, -0.67, 0.72, -2.14, 2.04), 4, 4, byrow = TRUE) eigjacobi(A)

# $V

# [,1] [,2] [,3] [,4]

# [1,] 0.87019414 -0.3151209 0.1975473 -0.3231656

# [2,] 0.11138094 0.8661855 0.1178032 -0.4726938

# [3,] 0.07043799 0.1683401 0.8273261 0.5312548

# [4,] 0.47475776 0.3494040 -0.5124734 0.6244140

# # $D

# [1] 0.66335457 3.39813189 5.58753257 0.02098098
```

einsteinF

Einstein Functions

### **Description**

Einstein functions.

# Usage

```
einsteinF(d, x)
```

# Arguments

```
x numeric or complex vector.
```

d parameter to select one of the Einstein functions E1, E2, E3, E4.

einsteinF 81

### **Details**

The Einstein functions are sometimes used for the Planck-Einstein oscillator in one degree of freedom

The functions are defined as:

$$E1(x) = \frac{x^2 e^x}{(e^x - 1)^2}$$

$$E2(x) = \frac{x}{e^x - 1}$$

$$E3(x) = \ln(1 - e^{-x})$$

$$E4(x) = \frac{x}{e^x - 1} - \ln(1 - e^{-x})$$

E1 has an inflection point as x=2.34694130...

### Value

Numeric/complex scalar or vector.

```
## Not run:
x1 < - seq(-4, 4, length.out = 101)
y1 \leftarrow einsteinF(1, x1)
plot(x1, y1, type = "l", col = "red",
            xlab = "", ylab = "", main = "Einstein Function E1(x)")
grid()
y2 \leftarrow einsteinF(2, x1)
plot(x1, y2, type = "1", col = "red",
            xlab = "", ylab = "", main = "Einstein Function E2(x)")
grid()
x3 < - seq(0, 5, length.out = 101)
y3 \leftarrow einsteinF(3, x3)
grid()
y4 \leftarrow einsteinF(4, x3)
plot(x3, y4, type = "1", col = "red",
            xlab = "", ylab = "", main = "Einstein Function E4(x)")
grid()
## End(Not run)
```

82 ellipke,ellipj

ellipke,ellipj

Elliptic and Jacobi Elliptic Integrals

### **Description**

Complete elliptic integrals of the first and second kind, and Jacobi elliptic integrals.

## Usage

```
ellipke(m, tol = .Machine$double.eps)
ellipj(u, m, tol = .Machine$double.eps)
```

### **Arguments**

u numeric vector.

m input vector, all input elements must satisfy  $0 \le x \le 1$ .

tol tolerance; default is machine precision.

### **Details**

ellipke computes the complete elliptic integrals to accuracy tol, based on the algebraic-geometric mean.

ellipj computes the Jacobi elliptic integrals sn, cn, and dn. For instance, sn is the inverse function for

$$u = \int_0^\phi dt / \sqrt{1 - m \sin^2 t}$$

with  $sn(u) = \sin(\phi)$ .

Some definitions of the elliptic functions use the modules k instead of the parameter m. They are related by  $k^2=m=\sin(a)^2$  where a is the 'modular angle'.

### Value

ellipke returns list with two components, k the values for the first kind, e the values for the second kind.

ellipj returns a list with components the three Jacobi elliptic integrals sn, cn, and dn.

#### References

Abramowitz, M., and I. A. Stegun (1965). Handbook of Mathematical Functions. Dover Publications, New York.

#### See Also

elliptic::sn,cn,dn

eps 83

### **Examples**

```
x \leftarrow linspace(0, 1, 20)
ke <- ellipke(x)</pre>
## Not run:
plot(x, ke\$k, type = "l", col = "darkblue", ylim = c(0, 5),
     main = "Elliptic Integrals")
lines(x, ke$e, col = "darkgreen")
legend( 0.01, 4.5,
        legend = c("Elliptic integral of first kind",
                   "Elliptic integral of second kind"),
        col = c("darkblue", "darkgreen"), lty = 1)
grid()
## End(Not run)
u \leftarrow c(0, 1, 2, 3, 4, 5)
m < - seq(0.0, 1.0, by = 0.2)
je <- ellipj(u, m)</pre>
# $sn
            0.0000 0.8265 0.9851 0.7433 0.4771 0.9999
            1.0000 0.5630 -0.1720 -0.6690 -0.8789 0.0135
# $cn
           1.0000 0.9292 0.7822 0.8176 0.9044 0.0135
# $dn
je$sn^2 + je$cn^2
                   # 1 1 1 1 1 1
je$dn^2 + m * je$sn^2 # 1 1 1 1 1 1
```

eps

Floating Point Relative Accuracy

# Description

Distance from 1.0 to the next largest double-precision number.

### Usage

```
eps(x = 1.0)
```

### **Arguments**

v

scalar or numerical vector or matrix.

### **Details**

d=eps(x) is the positive distance from abs(x) to the next larger floating point number in double precision.

If x is an array, eps(x) will return eps(max(abs(x))).

#### Value

Returns a scalar.

84 erf

### **Examples**

```
for (i in -5:5) cat(eps(10^i), "\n")
# 1.694066e-21
# 1.355253e-20
# 2.168404e-19
# 1.734723e-18
# 1.387779e-17
# 2.220446e-16
# 1.776357e-15
# 1.421085e-14
# 1.136868e-13
# 1.818989e-12
# 1.455192e-11
```

erf

Error Functions and Inverses (Matlab Style)

## **Description**

The error or Phi function is a variant of the cumulative normal (or Gaussian) distribution.

## Usage

```
erf(x)
erfinv(y)
erfc(x)
erfcinv(y)
erfcx(x)
erfz(z)
erfi(z)
```

# **Arguments**

```
x, y vector of real numbers.z real or complex number; must be a scalar.
```

### **Details**

```
erf and erfinv are the error and inverse error functions.
erfc and erfcinv are the complementary error function and its inverse.
erfcx is the scaled complementary error function.
erfz is the complex, erfi the imaginary error function.
```

## Value

Real or complex number(s), the value(s) of the function.

errorbar 85

## Note

For the complex error function we used Fortran code from the book S. Zhang & J. Jin "Computation of Special Functions" (Wiley, 1996).

### Author(s)

First version by Hans W Borchers; vectorized version of erfz by Michael Lachmann.

### See Also

pnorm

## **Examples**

```
x <- 1.0
erf(x); 2*pnorm(sqrt(2)*x) - 1
# [1] 0.842700792949715
# [1] 0.842700792949715
erfc(x); 1 - erf(x); 2*pnorm(-sqrt(2)*x)
# [1] 0.157299207050285
# [1] 0.157299207050285
# [1] 0.157299207050285
erfz(x)
# [1] 0.842700792949715
erfi(x)
# [1] 1.650425758797543</pre>
```

errorbar

Plot Error Bars

## **Description**

Draws symmetric error bars in x- and/or y-direction.

## Usage

## **Arguments**

x, y	x-, y-coordinates
xerr, yerr	length of the error bars, relative to the x-, y-values.
bar.col	color of the error bars; default: red
bar.len	length of the cross bars orthogonal to the error bars; default: 0.01.
grid	logical; should the grid be plotted?; default: true

86 eta

with	logical; whether to end the error bars with small cross bars.
add	logical; should the error bars be added to an existing plot?; default: false.
	additional plotting parameters that will be passed to the plot function.

#### **Details**

errorbar plots y versus x with symmetric error bars, with a length determined by xerr resp. yerr in x- and/or y-direction. If xerr or yerr is NULL error bars in this direction will not be drawn.

A future version will allow to draw unsymmetric error bars by specifying upper and lower limits when xerr or yerr is a matrix of size  $(2 \times length(x))$ .

### Value

Generates a plot, no return value.

## See Also

```
plotrix::plotCI, Hmisc::errbar
```

## **Examples**

```
## Not run:
x <- seq(0, 2*pi, length.out = 20)
y <- sin(x)
xe <- 0.1
ye <- 0.1 * y
errorbar(x, y, xe, ye, type = "l", with = FALSE)

cnt <- round(100*randn(20, 3))
y <- apply(cnt, 1, mean)
e <- apply(cnt, 1, sd)
errorbar(1:20, y, yerr = e, bar.col = "blue")

## End(Not run)</pre>
```

eta

Dirichlet Eta Function

# Description

Dirichlet's eta function valid in the entire complex plane.

## Usage

eta(z)

#### **Arguments**

z Real or complex number or a numeric or complex vector.

euler\_heun 87

### **Details**

Computes the eta function for complex arguments using a series expansion.

Accuracy is about 13 significant digits for abs(z)<100, drops off with higher absolute values.

### Value

Returns a complex vector of function values.

### Note

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#### References

Zhang, Sh., and J. Jin (1996). Computation of Special Functions. Wiley-Interscience, New York.

### See Also

```
gammaz, zeta
```

# Examples

```
z <- 0.5 + (1:5)*1i
eta(z)
z <- c(0, 0.5+1i, 1, 1i, 2+2i, -1, -2, -1-1i)
eta(z)
```

euler\_heun

Euler-Heun ODE Solver

# Description

Euler and Euler-Heun ODE solver.

## Usage

```
euler_heun(f, a, b, y0, n = 100, improved = TRUE, ...)
```

# Arguments

```
f function in the differential equation y' = f(x,y).

a, b start and end points of the interval.

y0 starting value at a.

n number of grid points.

improved logical; shall the Heun method be used; default TRUE.

... additional parameters to be passed to the function.
```

88 expint

### **Details**

euler\_heun is an integration method for ordinary differential equations using the simple Euler resp. the improved Euler-Heun Method.

#### Value

List with components t for grid (or 'time') points, and y the vector of predicted values at those grid points.

#### References

Quarteroni, A., and F. Saleri (). Scientific Computing with MATLAB and Octave. Second Edition, Springer-Verlag, Berlin Heidelberg, 2006.

### See Also

cranknic

### **Examples**

```
## Flame-up process
f <- function(x, y) y^2 - y^3
s1 <- cranknic(f, 0, 200, 0.01)
s2 <- euler_heun(f, 0, 200, 0.01)
## Not run:
plot(s1$t, s1$y, type="1", col="blue")
lines(s2$t, s2$y, col="red")
grid()
## End(Not run)</pre>
```

expint

Exponential and Logarithmic Integral

## **Description**

The exponential integral functions E1 and Ei and the logarithmic integral Li.

The exponential integral is defined for x > 0 as

$$\int_{T}^{\infty} \frac{e^{-t}}{t} dt$$

and by analytic continuation in the complex plane. It can also be defined as the Cauchy principal value of the integral

$$\int_{-\infty}^{x} \frac{e^{t}}{t} dt$$

This is denoted as Ei(x) and the relationship between Ei and expint(x) for x real, x > 0 is as follows:

$$Ei(x) = -E1(-x) - i\pi$$

expint 89

The logarithmic integral li(x) for real x, x > 0, is defined as

$$li(x) = \int_0^x \frac{dt}{log(t)}$$

and the Eulerian logarithmic integral as Li(x) = li(x) - li(2).

The integral Li approximates the prime number function  $\pi(n)$ , i.e., the number of primes below or equal to n (see the examples).

## Usage

```
expint(x)
expint_E1(x)
expint_Ei(x)
li(x)
```

### **Arguments**

Х

vector of real or complex numbers.

### **Details**

For x in [-38, 2] we use a series expansion, otherwise a continued fraction, see the references below, chapter 5.

### Value

Returns a vector of real or complex numbers, the vectorized exponential integral, resp. the logarithmic integral.

#### Note

The logarithmic integral li(10^i)-li(2) is an approximation of the number of primes below 10^i, i.e., Pi(10^i), see "?primes".

# References

Abramowitz, M., and I.A. Stegun (1965). Handbook of Mathematical Functions. Dover Publications, New York.

### See Also

```
gsl::expint_E1,expint_Ei,primes
```

90 expm

### **Examples**

```
expint_E1(1:10)
#  0.2193839  0.0489005  0.0130484  0.0037794  0.0011483
#  0.0003601  0.0001155  0.0000377  0.0000124  0.0000042
expint_Ei(1:10)

## Not run:
estimPi <- function(n) round(Re(li(n) - li(2))) # estimated number of primes
primesPi <- function(n) length(primes(n)) # true number of primes <= n
N <- 1e6
(estimPi(N) - primesPi(N)) / estimPi(N) # deviation is 0.16 percent!
## End(Not run)</pre>
```

expm

Matrix Exponential

### **Description**

Computes the exponential of a matrix.

## Usage

```
expm(A, np = 128)
logm(A)
```

### Arguments

A numeric square matrix.

np number of points to use on the unit circle.

## **Details**

For an analytic function f and a matrix A the expression f(A) can be computed by the Cauchy integral

 $f(A) = (2\pi i)^{-1} \int_{G} (zI - A)^{-1} f(z) dz$ 

where G is a closed contour around the eigenvalues of A.

Here this is achieved by taking G to be a circle and approximating the integral by the trapezoid rule.

logm is a fake at the moment as it computes the matrix logarithm through taking the logarithm of its eigenvalues; will be replaced by an approach using Pade interpolation.

Another more accurate and more reliable approach for computing these functions can be found in the R package 'expm'.

### Value

Matrix of the same size as A.

expm 91

## Note

This approach could be used for other analytic functions, but a point to consider is which branch to take (e.g., for the logm function).

#### Author(s)

Idea and Matlab code for a cubic root by Nick Trefethen in his "10 digits 1 page" project, for realization see file 'cuberootA.m' at http://people.maths.ox.ac.uk/trefethen/tda.html.

#### References

Moler, C., and Ch. Van Loan (2003). Nineteen Dubious Ways to Compute the Exponential of a Matrix, Twenty-Five Years Later. SIAM Review, Vol. 1, No. 1, pp. 1–46. [Available at CiteSeer, citeseer.ist.psu.edu]

N. J. Higham (2008). Matrix Functions: Theory and Computation. SIAM Society for Industrial and Applied Mathematics.

#### See Also

```
expm::expm
```

```
## The Ward test cases described in the help for expm::expm agree up to
## 10 digits with the values here and with results from Matlab's expm !
A \leftarrow matrix(c(-49, -64, 24, 31), 2, 2)
expm(A)
# -0.7357588 0.5518191
# -1.4715176 1.1036382
A1 <- matrix(c(10, 7, 8, 7,
                7, 5, 6, 5,
                8, 6, 10, 9,
                7, 5, 9, 10), nrow = 4, ncol = 4, byrow = TRUE)
expm(logm(A1))
logm(expm(A1))
## System of linear differential equations: y' = M y \quad (y = c(y1, y2, y3))
M \leftarrow matrix(c(2,-1,1, 0,3,-1, 2,1,3), 3, 3, byrow=TRUE)
C1 <- 0.5; C2 <- 1.0; C3 <- 1.5
t <- 2.0; Mt <- expm(t * M)
yt <- Mt
```

92 ezcontour,ezmesh

eye

Some Basic Matrices

# Description

Create basic matrices.

### Usage

```
eye(n, m = n)
ones(n, m = n)
zeros(n, m = n)
```

# Arguments

m, n

numeric scalars specifying size of the matrix

### Value

Matrix of size  $n \times m$ . Defaults to a square matrix if m is missing.

No dropping of dimensions; if n = 1, still returns a matrix and not a vector.

## See Also

Diag,

# **Examples**

```
eye(3)
ones(3, 1)
zeros(1, 3)
```

ezcontour, ezmesh

Contour and Mesh Plotter

## **Description**

Easy-to-use contour and 3-D mesh plotter.

### Usage

```
ezcontour(f, xlim = c(-pi,pi), ylim = c(-pi,pi),

n = 60, filled = FALSE, col = NULL)

ezmesh(f, xlim = c(-pi,pi), ylim = c(-pi,pi),

n = 60, col = "lightgray", ...)
```

ezcontour,ezmesh 93

### Arguments

```
f 2-D function to be plotted, must accept (x,y) as a vector.
xlim, ylim defines x- and y-ranges as intervals.

n number of grid points in each direction.

col colour of isolines lines, resp. the surface color.

filled logical; shall the contour plot be

... parameters to be passed to the persp function.
```

### **Details**

ezcontour generates a contour plot of the function f using contour (and image if filled=TRUE is chosen). If filled=TRUE is chosen, col should be a color scheme, the default is heat.colors(12).

ezmesh generates a mesh/surface plot of the function f using persp. The most important additional parameters to be passed in . . . are and .

The function f needs not be vectorized in any form.

#### Value

Plots the function graph and invisibly returns NULL.

### Note

Mimicks Matlab functions of the same names; Matlab's ezcontourf can be generated with filled=TRUE.

## See Also

```
contour, image, persp
```

```
## Not run:
f <- function(xy) {
    x <- xy[1]; y <- xy[2]
    3*(1-x)^2 * exp(-(x^2) - (y+1)^2) -
        10*(x/5 - x^3 - y^5) * exp(-x^2 - y^2) -
        1/3 * exp(-(x+1)^2 - y^2)
    }
ezcontour(f, col = "navy")
ezcontour(f, filled = TRUE)
ezmesh(f)
ezmesh(f, col="lightblue", theta = -15, phi = 30)
## End(Not run)</pre>
```

94 ezplot

ezplot	Easy Function Plot	

# Description

Easy function plot/wo the need to define x, y coordinates.

## Usage

### **Arguments**

f	Function to be plotted.
a, b	Left and right endpoint for the plot.
n	Number of points to plot.
col	Color of the function graph.
add	logical; shall the polt be added to an existing plot.
lty	line type; default 1.
lwd	line width; default 1.
marker	no. of markers to be added to the curve; defailt: none.
pch	poimt character; default circle.
grid	Logical; shall a grid be plotted?; default TRUE.
gridcol	Color of grid points.
fill	$Logical; shall \ the \ area \ between \ function \ and \ axis \ be \ filled?; \ default: \ {\tt FALSE}.$
fillcol	Color of fill area.
xlab	Label on the x-axis.
ylab	Label on the y-axis.
main	Title of the plot
	More parameters to be passed to plot.

### **Details**

Calculates the x, y coordinates of points to be plotted and calls the plot function.

If fill is TRUE, also calls the polygon function with the x, y coordinates in appropriate order.

If the no. of markers is greater than 2, this number of markers will be added to the curve, with equal distances measured along the curve.

ezpolar 95

## Value

Plots the function graph and invisibly returns NULL.

#### Note

Should mimick the Matlab function of the same name, has some more functionality, misses the possibility to plot several functions.

## See Also

curve

## **Examples**

```
## Not run:
fun <- function(x) x * cos(0.1*exp(x)) * sin(0.1*pi*exp(x))
ezplot(fun, 0, 5, n = 1001, fill = TRUE)
## End(Not run)</pre>
```

ezpolar

Easy Polar Plot

# Description

Easy function plot w/o the need to define x, y coordinates.

## Usage

```
ezpolar(fun, interv = c(0, 2*pi))
```

# Arguments

fun function to be plotted.

interv left and right endpoint for the plot.

## **Details**

Calculates the x, y coordinates of points to be plotted and calls the polar function.

## Value

Plots the function graph and invisibly returns NULL.

### Note

Mimick the Matlab function of the same name.

96 fact

## See Also

```
ezplot
```

## **Examples**

```
## Not run:
fun <- function(x) 1 + cos(x)
ezpolar(fun)
## End(Not run)</pre>
```

fact

Factorial Function

# Description

Factorial for non-negative integers  $n \le 170$ .

### Usage

fact(n)

## **Arguments**

n

Vector of integers.

## **Details**

The factorial is computed by brute force; factorials for  $n \ge 171$  are not representable as 'double' anymore.

### Value

Returns the factorial of each element in n. If  $n < \emptyset$  the value is NaN, and for n > 170 it is Inf. Non-integers will be reduced to integers through floor(n).

# Note

The R core function factorial uses the gamma function, whose implementation is not accurate enough for larger input values.

### See Also

factorial

factors 97

### **Examples**

```
fact(c(-1, 0, 1, NA, 171)) #=> NaN 1 1 NA Inf
fact(100) #=> 9.332621544394410e+157
factorial(100) #=> 9.332621544394225e+157
# correct value: 9.332621544394415e+157
# Stirling's approximation: 9.324847625269420e+157
# n! ~ sqrt(2*pi*n) * (n/e)^n
```

factors

Prime Factors

## Description

Returns a vector containing the prime factors of n.

### Usage

```
factors(n)
```

## **Arguments**

n

nonnegative integer

# **Details**

Computes the prime factors of n in ascending order, each one as often as its multiplicity requires, such that n == prod(factors(n)).

The corresponding Matlab function is called 'factor', but because factors have a special meaning in R and the factor() function in R could not (or should not) be shadowed, the number theoretic function has been renamed here.

### Value

Vector containing the prime factors of n.

### See Also

```
isprime, primes
```

```
## Not run:
  factors(1002001)  # 7 7 11 11 13 13
  factors(65537)  # is prime
  # Euler's calculation
  factors(2^32 + 1)  # 641 6700417
## End(Not run)
```

98 fderiv

fderiv Numerical Differentiation
----------------------------------

### **Description**

Numerical function differentiation for orders n=1..4 using finite difference approximations.

## Usage

```
fderiv(f, x, n = 1, h = 0, method = c("central", "forward", "backward"), ...)
```

## Arguments

f	function to be differentiated.
х	point(s) where differentiation will take place.
n	order of derivative, should only be between 1 and 8; for $n=0$ function values will be returned.
h	step size: if h=0 step size will be set automatically.
method	one of "central", "forward", or "backward".
	more variables to be passed to function f.

#### **Details**

Derivatives are computed applying central difference formulas that stem from the Taylor series approximation. These formulas have a convergence rate of  $O(h^2)$ .

Use the 'forward' (right side) or 'backward' (left side) method if the function can only be computed or is only defined on one side. Otherwise, always use the central difference formulas.

Optimal step sizes depend on the accuracy the function can be computed with. Assuming internal functions with an accuracy 2.2e-16, appropriate step sizes might be 5e-6, 1e-4, 5e-4, 2.5e-3 for  $n=1,\ldots,4$  and precisions of about  $10^{-10}$ ,  $10^{-8}$ ,  $5*10^{-7}$ ,  $5*10^{-6}$  (at best).

For n>4 a recursion (or finite difference) formula will be applied, cd. the Wikipedia article on "finite difference".

### Value

Vector of the same length as x.

### Note

Numerical differentiation suffers from the conflict between round-off and truncation errors.

### References

Kiusalaas, J. (2005). Numerical Methods in Engineering with Matlab. Cambridge University Press.

fibsearch 99

### See Also

```
numderiv, taylor
```

### **Examples**

```
## Not run:
f <- sin
xs <- seq(-pi, pi, length.out = 100)</pre>
ys \leftarrow f(xs)
y1 \leftarrow fderiv(f, xs, n = 1, method = "backward")
y2 \leftarrow fderiv(f, xs, n = 2, method = "backward")
y3 <- fderiv(f, xs, n = 3, method = "backward")
y4 <- fderiv(f, xs, n = 4, method = "backward")
plot(xs, ys, type = "1", col = "gray", lwd = 2,
     xlab = "", ylab = "", main = "Sinus and its Derivatives")
lines(xs, y1, col=1, lty=2)
lines(xs, y2, col=2, lty=3)
lines(xs, y3, col=3, lty=4)
lines(xs, y4, col=4, lty=5)
grid()
## End(Not run)
```

fibsearch

Fibonacci Search

## **Description**

Fibonacci search for function minimum.

## Usage

```
fibsearch(f, a, b, ..., endp = FALSE, tol = .Machine$double.eps^(1/2)$)
```

## **Arguments**

```
f Function or its name as a string.

a, b endpoints of the interval

endp logical; shall the endpoints be considered as possible minima?

tol absolute tolerance; default eps^(1/2).

Additional arguments to be passed to f.
```

#### **Details**

Fibonacci search for a univariate function minimum in a bounded interval.

100 figure

### Value

Return a list with components xmin, fmin, the function value at the minimum, niter, the number of iterations done, and the estimated precision estim.prec

#### See Also

uniroot

## **Examples**

```
f <- function(x) x * cos(0.1*exp(x)) * sin(0.1*pi*exp(x)) fibsearch(f, 0, 4, tol=10^-10) # $xmin = 3.24848329403424 optimize(f, c(0,4), tol=10^-10) # $minimum = 3.24848328971188
```

figure

Control Plot Devices (Matlab Style)

## Description

Open, activate, and close grahics devices.

### Usage

```
figure(figno, title = "")
```

### **Arguments**

figno (single) number of plot device. title title of the plot device; not yet used.

### **Details**

The number of a graphics device cannot be 0 or 1. The function will work for the operating systems Mac OS, MS Windows, and most Linux systems.

If figno is negative and a graphics device with that number does exist, it will be closed.

#### Value

No return value, except when a device of that number does not exist, in which case it returns a list of numbers of open graphics devices.

## Note

Does not bring the activated graphics device in front.

#### See Also

```
dev.set, dev.off, dev.list
```

findintervals 101

## **Examples**

```
## Not run:
figure()
figure(-2)
## End(Not run)
```

findintervals

Find Interval Indices

# Description

Find indices i in vector xs such that either x=xs[i] or such that xs[i]<x<xs[i+1] or xs[i]>x>xs[i+1].

## Usage

```
findintervals(x, xs)
```

# Arguments

x single number.

xs numeric vector, not necessarily sorted.

## **Details**

Contrary to findInterval, the vector xs in findintervals need not be sorted.

#### Value

Vector of indices in 1..length(xs). If none is found, returns integer(0).

### Note

If x is equal to the last element in xs, the index length(xs) will also be returned.

```
xs <- zapsmall(sin(seq(0, 10*pi, len=100)))
findintervals(0, xs)
# 1 10 20 30 40 50 60 70 80 90 100</pre>
```

102 findmins

findmins

Find All Minima

#### **Description**

Finding all local(!) minima of a unvariate function in an interval by splitting the interval in many small subintervals.

### Usage

```
findmins(f, a, b, n = 100, tol = .Machine$double.eps^(2/3), ...)
```

### **Arguments**

f	functions whose minima shall be found.
a, b	endpoints of the interval.
n	number of subintervals to generate and search.
tol	has no effect at this moment.
	Additional parameters to be passed to the function.

#### **Details**

Local minima are found by looking for one minimum in each subinterval. It will be found by applying optimize to any two adjacent subinterval where the first slope is negative and the second one positive.

If the function is minimal on a whole subinterval, this will cause problems. If some minima are apparently not found, increase the number of subintervals.

Note that the endpoints of the interval will never be considered to be local minima. The function need not be vectorized.

#### Value

Numeric vector with the x-positions of all minima found in the interval.

## See Also

```
optimize
```

```
fun <- function(x) x * cos(0.1*exp(x)) * sin(0.1*pi*exp(x))
## Not run: ezplot(fun, 0, 5, n = 1001)

# If n is smaller, the rightmost minimum will not be found.
findmins(fun, 0, 5, n= 1000)
# 2.537727 3.248481 3.761840 4.023021 4.295831
# 4.455115 4.641481 4.756263 4.897461 4.987802</pre>
```

findpeaks 103

|--|

# Description

Find peaks (maxima) in a time series.

# Usage

## **Arguments**

X	numerical vector taken as a time series
nups	minimum number of increasing steps before a peak is reached
ndowns	minimum number of decreasing steps after the peak
zero	can be $^{\prime}+^{\prime}, ^{\prime}-^{\prime},$ or $^{\prime}0^{\prime};$ how to interprete succeeding steps of the same value: increasing, decreasing, or special
peakpat	define a peak as a regular pattern, such as the default pattern " $[+]1,[-]1,$ "; if a pattern is provided, the parameters nups and ndowns are not taken into account
minpeakheight	the minimum (absolute) height a peak has to have to be recognized as such
minpeakdistance	2
	the minimum distance (in indices) peaks have to have to be counted
threshold	the minimum
npeaks	the number of peaks to return
sortstr	logical; should the peaks be returned sorted in decreasing oreder of their maximum value

# **Details**

This function is quite general as it relies on regular patterns to determine where a peak is located, from beginning to end.

## Value

Returns a matrix where each row represents one peak found. The first column gives the height, the second the position/index where the maximum is reached, the third and forth the indices of where the peak begins and ends — in the sense of where the pattern starts and ends.

104 finds

### Note

On Matlab Central there are several realizations for finding peaks, for example "peakfinder", "peak-seek", or "peakdetect". And "findpeaks" is also the name of a function in the Matlab 'signal' toolbox.

The parameter names are taken from the "findpeaks" function in 'signal', but the implementation utilizing regular expressions is unique and fast.

#### See Also

hampel

### **Examples**

```
x <- seq(0, 1, len = 1024)
pos <- c(0.1, 0.13, 0.15, 0.23, 0.25, 0.40, 0.44, 0.65, 0.76, 0.78, 0.81)
hgt <- c(4, 5, 3, 4, 5, 4.2, 2.1, 4.3, 3.1, 5.1, 4.2)
wdt <- c(0.005, 0.005, 0.006, 0.01, 0.01, 0.03, 0.01, 0.01, 0.005, 0.008, 0.005)

pSignal <- numeric(length(x))
for (i in seq(along=pos)) {
   pSignal <- pSignal + hgt[i]/(1 + abs((x - pos[i])/wdt[i]))^4
}
findpeaks(pSignal, npeaks=3, threshold=4, sortstr=TRUE)

## Not run:
plot(pSignal, type="l", col="navy")
grid()
x <- findpeaks(pSignal, npeaks=3, threshold=4, sortstr=TRUE)
points(x[, 2], x[, 1], pch=20, col="maroon")
## End(Not run)</pre>
```

finds

find function (Matlab Style)

## **Description**

Finds indices of nonzero elements.

### Usage

finds(v)

### Arguments

v

logical or numeric vector or array

#### **Details**

Finds indices of true or nonzero elements of argument v; can be used with a logical expression.

findzeros 105

### Value

Indices of elements matching the expression x.

## **Examples**

```
finds(-3:3 \ge 0)
finds(c(0, 1, 0, 2, 3))
```

findzeros

Find All Roots

# Description

Finding all roots of a unvariate function in an interval by splitting the interval in many small subintervals.

## Usage

```
findzeros(f, a, b, n = 100, tol = .Machinesdouble.eps^(2/3), ...)
```

#### **Arguments**

f functions whose roots shall be found.

a, b endpoints of the interval.

n number of subintervals to generate and search.

tol tolerance for identifying zeros.

... Additional parameters to be passed to the function.

## **Details**

Roots, i.e. zeros in a subinterval will be found by applying uniroot to any subinterval where the sign of the function changes. The endpoints of the interval will be tested separately.

If the function points are both positive or negative and the slope in this interval is high enough, the minimum or maximum will be determined with optimize and checked for a possible zero.

The function need not be vectorized.

### Value

Numeric vector with the x-positions of all roots found in the interval.

#### See Also

findmins

106 fletcher-powell

### **Examples**

```
f1 <- function(x) sin(pi/x)</pre>
findzeros(f1, 1/10, 1)
# 0.1000000 0.1111028 0.1250183 0.1428641 0.1666655
# 0.2000004 0.2499867 0.3333441 0.4999794 1.0000000
f2 <- function(x) 0.5*(1 + sin(10*pi*x))
findzeros(f2, 0, 1)
# 0.15 0.35 0.55 0.75 0.95
f3 \leftarrow function(x) sin(pi/x) + 1
findzeros(f3, 0.1, 0.5)
# 0.1052632 0.1333333 0.1818182 0.2857143
f4 \leftarrow function(x) sin(pi/x) - 1
findzeros(f4, 0.1, 0.5)
# 0.1176471 0.1538462 0.2222222 0.4000000
## Not run:
# Dini function
Dini <- function(x) x * besselJ(x, 1) + 3 * besselJ(x, 0)
findzeros(Dini, 0, 100, n = 128)
ezplot(Dini, 0, 100, n = 512)
## End(Not run)
```

fletcher-powell

Davidon-Fletcher-Powell Method

### **Description**

Davidon-Fletcher-Powell method for function minimization.

The Davidon-Fletcher-Powell (DFP) and the Broyden-Fletcher-Goldfarb-Shanno (BFGS) methods are the first quasi-Newton minimization methods developed. These methods differ only in some details; in general, the BFGS approach is more robust.

## Usage

```
fletcher_powell(x0, f, g = NULL,

maxiter = 1000, tol = .Machine$double.eps^(2/3)$)
```

## Arguments

x0	start	value.
A 0	start	varuc.

f function to be minimized.

g gradient function of f; if NULL, a numerical gradient will be calculated.

maxiter max. number of iterations.

tol relative tolerance, to be used as stopping rule.

fletcher-powell 107

### **Details**

The starting point is Newton's method in the multivariate case, when the estimate of the minimum is updated by the following equation

$$x_{new} = x - H^{-1}(x)grad(g)(x)$$

where H is the Hessian and grad the gradient.

The basic idea is to generate a sequence of good approximations to the inverse Hessian matrix, in such a way that the approximations are again positive definite.

## Value

List with following components:

minimum solution found.
fmin value of f at minimum.

niter number of iterations performed.

#### Note

Used some Matlab code as described in the book "Applied Numerical Analysis Using Matlab" by L. V.Fausett.

#### References

J. F. Bonnans, J. C. Gilbert, C. Lemarechal, and C. A. Sagastizabal. Numerical Optimization: Theoretical and Practical Aspects. Second Edition, Springer-Verlag, Berlin Heidelberg, 2006.

### See Also

```
steep_descent
```

```
## Rosenbrock function
rosenbrock <- function(x) {
    n <- length(x)
    x1 <- x[2:n]
    x2 <- x[1:(n-1)]
    sum(100*(x1-x2^2)^2 + (1-x2)^2)
}
fletcher_powell(c(0, 0), rosenbrock)
# $xmin
# [1] 1 1
# $fmin
# [1] 1.774148e-27
# $niter
# [1] 14</pre>
```

108 flipdim

flipdim

Matrix Flipping (Matlab Style)

# Description

Flip matrices up and down or left and right; or circulating indices per dimension.

## Usage

```
flipdim(a, dim)
flipud(a)
fliplr(a)
circshift(a, sz)
```

# **Arguments**

```
a numeric or complex matrix

dim flipping dimension; can only be 1 (default) or 2

sz integer vector of length 1 or 2.
```

### **Details**

flipdim will flip a matrix along the dim dimension, where dim=1 means flipping rows, and dim=2 flipping the columns.

```
flipud and fliplr are simply shortcuts for flipdim(a, 1) resp. flipdim(a, 2). circshift(a, sz) circulates each dimension (should be applicable to arrays).
```

## Value

the original matrix somehow flipped or circularly shifted.

```
a <- matrix(1:12, nrow=3, ncol=4, byrow=TRUE)
flipud(a)
fliplr(a)

circshift(a, c(1, -1))
v <- 1:10
circshift(v, 5)</pre>
```

fminbnd 109

fminbnd	Finding Function Minimum
---------	--------------------------

### **Description**

Find minimum of single-variable function on fixed interval.

## Usage

```
fminbnd(f, a, b, maxiter = 1000, maximum = FALSE,
            tol = 1e-07, rel.tol = tol, abs.tol = 1e-15, ...)
```

#### Arguments

f function whose minimum or maximum is to be found.

a, b endpoints of the interval to be searched.

maxiter maximal number of iterations.

maximum logical; shall maximum or minimum be found; default FALSE.

tol relative tolerance; left over for compatibility.

rel.tol, abs.tol

relative and absolute tolerance.

... additional variables to be passed to the function.

## **Details**

fminbnd finds the minimum of a function of one variable within a fixed interval. It applies Brent's algorithm, based on golden section search and parabolic interpolation.

fminbnd may only give local solutions. fminbnd never evaluates f at the endpoints.

### Value

### List with

xmin location of the minimum resp. maximum.

fmin function value at the optimum.

niter number of iterations used.

estim.prec estimated precision.

#### Note

fminbnd mimics the Matlab function of the same name.

### References

R. P. Brent (1973). Algorithms for Minimization Without Derivatives. Dover Publications, reprinted 2002.

110 fminsearch

### See Also

```
fibsearch, golden_ratio
```

## **Examples**

```
## CHEBFUN example by Trefethen f \leftarrow function(x) \exp(x) * \sin(3*x) * \tanh(5*\cos(30*x)) fminbnd(f, -1, 1) # fourth local minimum (from left) g \leftarrow function(x) = func
```

fminsearch

Minimum Finding

## **Description**

Find minimum of unconstrained multivariable function.

### Usage

### **Arguments**

f	function whose minimum or maximum is to be found.
x0	point considered near to the optimum.
minimize	logical; shall a minimum or a maximum be found.
dfree	logical; apply derivative-free optimization or not.
maxiter	maximal number of iterations
tol	relative tolerance.
	additional variables to be passed to the function.

fminsearch 111

## **Details**

fminsearch finds the minimum of a nonlinear scalar multivariable function, starting at an initial estimate and returning a value x that is a local minimizer of the function.

With minimize=FALSE it seaches for a maximum. dfree=TRUE applies Nelder.Mead, else Fletcher-Powell, calculating the derivatives numerically.

This is generally referred to as unconstrained nonlinear optimization. fminsearch may only give local solutions.

## Value

List with

xopt location of the location of minimum resp. maximum.

fval function value at the optimum.

niter number of iterations.

## Note

fminbnd mimics the Matlab function of the same name.

### References

Nocedal, J., and S. Wright (2006). Numerical Optimization. Second Edition, Springer-Verlag, New York.

## See Also

optim

```
# Rosenbrock function rosena <- function(x, a) 100*(x[2]-x[1]^2)^2 + (a-x[1])^2 # min: (a, a^2) fminsearch(rosena, c(-1.2, 1), a = sqrt(2)) # x = (1.414214 2.000010) , fval = 1.239435e-11 fminsearch(rosena, c(-1.2, 1), dfree=FALSE, a = sqrt(2)) # x = (1.414214 2.000000) , fval = 3.844519e-26
```

112 fnorm

fnorm Function Norm
---------------------

## **Description**

The fnorm function calculates several different types of function norms for depending on the argument p.

# Usage

```
fnorm(f, g, x1, x2, p = 2, npoints = 100)
```

# **Arguments**

f, g	functions given by name or string.
x1, x2	endpoints of the interval.
p	Numeric scalar or Inf, -Inf; default is 2.
npoints	number of points to be considered in the interval.

## **Details**

fnorm returns a scalar that gives some measure of the distance of two functions f and g on the interval [x1, x2].

It takes npoints equidistant points in the interval, computes the function values for f and g and applies Norm to their difference.

Especially p=Inf returns the maximum norm, while fnorm(f, g, x1, x2, p=1, npoints) / npoints would return some estimate of the mean distance.

### Value

Numeric scalar (or Inf), or NA if one of these functions returns NA.

## Note

Another kind of 'mean' distance could be calculated by integrating the difference f-g and dividing through the length of the interval.

### See Also

Norm

fornberg 113

### **Examples**

```
xp <- seq(-1, 1, length.out = 6)
yp <- runge(xp)
p5 <- polyfit(xp, yp, 5)
f5 <- function(x) polyval(p5, x)
fnorm(runge, f5, -1, 1, p = Inf)  #=> 0.4303246
fnorm(runge, f5, -1, 1, p = Inf, npoints = 1000) #=> 0.4326690

# Compute mean distance using fnorm:
fnorm(runge, f5, -1, 1, p = 1, 1000) / 1000 #=> 0.1094193

# Compute mean distance by integration:
fn <- function(x) abs(runge(x) - f5(x))
integrate(fn, -1, 1)$value / 2 #=> 0.1095285
```

fornberg

Fornberg's Finite Difference Approximation

### **Description**

Finite difference approximation using Fornberg's method for the derivatives of order 1 to k based on irregulat grid values.

### Usage

```
fornberg(x, y, xs, k = 1)
```

### **Arguments**

X	grid points on the x-axis, must be distinct.
У	discrete values of the function at the grid points.
xs	point at which to approximate (not vectorized).
k	order of derivative, $k \le length(x) - 1$ required.

#### **Details**

Compute coefficients for finite difference approximation for the derivative of order k at xs based on grid values at points in x. For k=0 this will evaluate the interpolating polynomial itself, but call it with k=1.

### Value

Returns a matrix of size (length(xs)), where the (k+1)-th column gives the value of the k-th derivative. Especially the first column returns the polynomial interpolation of the function.

114 fplot

## Note

Fornberg's method is considered to be numerically more stable than applying Vandermonde's matrix.

#### References

LeVeque, R. J. (2007). Finite Difference Methods for Ordinary and Partial Differential Equations. Society for Industrial and Applied Mathematics (SIAM), Philadelphia.

### See Also

```
neville, newtonInterp
```

# **Examples**

```
x <- 2 * pi * c(0.0, 0.07, 0.13, 0.2, 0.28, 0.34, 0.47, 0.5, 0.71, 0.95, 1.0)
y <- sin(0.9*x)
xs <- linspace(0, 2*pi, 51)
fornb <- fornberg(x, y, xs, 10)
## Not run:
matplot(xs, fornb, type="l")
grid()
## End(Not run)</pre>
```

fplot

Plot Multivariate Function

# Description

Plots components of a (multivariate) function between the specifies limits.

# Usage

## **Arguments**

Ť	multivariate function, vectorized or not.
a, b	begin and end of the interval.
n	number of grid points.
vectorized	logical; is the function vectorized (in column form)?)
col	vector of colors; default 1:8
lty	vector of line types.
lwd	vector of line widths.
	more parameters to be passed to the plotting routine.

fresnelS/C 115

## **Details**

The function must be of the form y=f(x), where x is a vector whose range fulfills the limits, and y is a vector. If the function returns more than one value for a given x, then y is a matrix whose columns contain each component of f(x).

For example, if f(x) returns (f1(x), f2(x), f3(x)) then for input (x1, x2) the function should return the matrix

```
f1(x1) f2(x1) f3(x1)
f1(x2) f2(x2) f3(x2)
```

At least, this is assumed when vectorized=TRUE. If this is not the case or it turns out that size(f(c(a,b)), 1) is not 2, then this function matrix will be generated in a loop.

### Value

A graph, no return value.

#### Note

matplot will plot the graph if the matrix is already generated.

### See Also

```
matplot
```

### **Examples**

```
## Not run:
f <- function(x) cbind(x, x^2, x^3, x^4, x^5, x^6, x^7, x^8)
fplot(f, 0, 1)
## End(Not run)</pre>
```

fresnelS/C

Fresnel Integrals

### **Description**

```
(Normalized) Fresnel integrals S(x) and C(x)
```

## Usage

```
fresnelS(x) fresnelC(x)
```

## **Arguments**

Χ

numeric vector.

116 fresnelS/C

### **Details**

The normalized Fresnel integrals are defined as

$$S(x) = \int_0^x \sin(\pi/2t^2)dt$$

$$C(x) = \int_0^x \cos(\pi/2t^2)dt$$

This program computes the Fresnel integrals S(x) and C(x) using Fortran code by Zhang and Jin. The accuracy is almost up to Machine precision.

The functions are not (yet) truly vectorized, but use a call to 'apply'. The underlying function fresnel (not exported) computes single values of S(x) and C(x) at the same time.

### Value

Numeric vector of function values.

### Note

Copyright (c) 1996 Zhang and Jin for the Fortran routines, converted to Matlab using the open source project 'f2matlab' by Ben Barrowes, posted to MatlabCentral in 2004, and then translated to R by Hans W. Borchers.

#### References

Zhang, S., and J. Jin (1996). Computation of Special Functions. Wiley-Interscience.

## See Also

gaussLegendre

```
## Compute Fresnel integrals through Gauss-Legendre quadrature
f1 <- function(t) sin(0.5 * pi * t^2)
f2 <- function(t) cos(0.5 * pi * t^2)
for (x in seq(0.5, 2.5, by = 0.5)) {
    cgl <- gaussLegendre(51, 0, x)
    fs <- sum(cgl$w * f1(cgl$x))
    fc <- sum(cgl$w * f2(cgl$x))
    cat(formatC(c(x, fresnelS(x), fs, fresnelC(x), fc),
        digits = 8, width = 12, flag = " ----"), "\n")
}

## Not run:
xs <- seq(0, 7.5, by = 0.025)
ys <- fresnelS(xs)
yc <- fresnelC(xs)

## Function plot of the Fresnel integrals</pre>
```

fsolve 117

fsolve

Solve System of Nonlinear Equations

### **Description**

Solve a system of m nonlinear equations of n variables.

### Usage

## Arguments

f function describing the system of equations.

x0 point near to the root.

J Jacobian function of f, or NULL.

maxiter maximum number of iterations in gaussNewton.

tol tolerance to be used in Gauss-Newton.

... additional variables to be passed to the function.

### **Details**

fsolve tries to solve the components of function f simultaneously and uses the Gauss-Newton method with numerical gradient and Jacobian. If m = n, it uses broyden.

# Value

List with

x location of the solution.

fval function value at the solution.

118 fzero

### Note

fsolve mimics the Matlab function of the same name.

#### References

Antoniou, A., and W.-S. Lu (2007). Practical Optimization: Algorithms and Engineering Applications. Springer Science+Business Media, New York.

### See Also

broyden, gaussNewton

## **Examples**

```
## Not run:
# Find a matrix X such that X * X * X = [1, 2; 3, 4]
F <- function(x) {
    a <- matrix(c(1, 3, 2, 4), nrow = 2, ncol = 2, byrow = TRUE)
    X <- matrix(x, nrow = 2, ncol = 2, byrow = TRUE)
    return(c(X %*% X %*% X - a))
}
x0 <- matrix(1, 2, 2)
X <- matrix(fsolve(F, x0)$x, 2, 2)
X
# -0.1291489    0.8602157
#    1.2903236    1.1611747
## End(Not run)</pre>
```

fzero

Root Finding

### **Description**

Find root of continuous function of one variable.

## Usage

```
fzero(f, x, ..., maxiter = 100, tol = .Machine$double.eps^(1/2))
```

### **Arguments**

```
f function whose root is sought.

x a point near the root or an interval giving end points.

maxiter maximum number of iterations.

tol relative tolerance.

... additional arguments to be passed to the function.
```

fzsolve 119

### **Details**

fzero tries to find a zero of f near x, if x is a scalar. Expands the interval until different signs are found at the endpoints or the maximum number of iterations is exceeded. If x is a vector of length two, fzero assumes x is an interval where the sign of x[1] differs from the sign of x[1]. An error occurs if this is not the case.

"This is essentially the ACM algorithm 748. The structure of the algorithm has been transformed non-trivially: it implement here a FSM version using one interior point determination and one bracketing per iteration, thus reducing the number of temporary variables and simplifying the structure."

This approach will not find zeroes of quadratic order.

#### Value

fzero returns a list with

x location of the root. fval function value at the root.

#### Note

fzero mimics the Matlab function of the same name, but is translated from Octave's fzero function, copyrighted (c) 2009 by Jaroslav Hajek.

#### References

Alefeld, Potra and Shi (1995). Enclosing Zeros of Continuous Functions. ACM Transactions on Mathematical Software, Vol. 21, No. 3.

# See Also

```
uniroot, brent
```

## **Examples**

```
fzero(sin, 3) # 3.141593
fzero(cos,c(1, 2)) # 1.570796
fzero(function(x) x^3-2*x-5, 2) # 2.094551
```

fzsolve

Complex Root Finding

### **Description**

Find the root of a complex function

#### Usage

```
fzsolve(fz, z0)
```

120 gammainc

# Arguments

fz	complex(-analytic) function.

z0 complex point near the assumed root.

### **Details**

fzsolve tries to find the root of the complex and relatively smooth (i.e., analytic) function near a starting point.

The function is considered as real function R^2 --> R^2 and the newtonsys function is applied.

### Value

Complex point with sufficiently small function value.

### See Also

```
newtonsys
```

# **Examples**

```
fz <- function(z) sin(z)^2 + sqrt(z) - log(z)
fzsolve(fz, 1+1i)
# 0.2555197+0.8948303i</pre>
```

gammainc

Incomplete Gamma Function

# Description

Lower and upper incomplete gamma function.

## Usage

```
gammainc(x, a)
```

# **Arguments**

- x real number, not too big.
- a real positive number.

gammaz 121

### **Details**

Computes the lower and upper incomplete gamma function, including the regularized gamma function. The lower and upper incomplete gamma functions are defined as

$$\gamma(x,a) = \int_0^x e^{-t} t^{a-1} dt$$

and

$$\Gamma(x,a) = \int_{x}^{\infty} e^{-t} t^{a-1} dt$$

while the regularized incomplete gamma function is  $\gamma(x,a)/\Gamma(a)$ .

Accuracy is 7 significant digits along the real axis.

#### Value

Returns a list with the values of the lower, the upper, and regularized lower incomplete gamma function.

#### Note

Directly converting Fortran code is often easier than translating Matlab code generated with f2matlab.

#### References

Zhang, Sh., and J. Jin (1996). Computation of Special Functions. Wiley-Interscience, New York.

#### See Also

gamma

# Examples

```
gammainc( 1.5, 2)
gammainc(-1.5, 2)
```

gammaz

Complex Gamma Function

# Description

Gamma function valid in the entire complex plane.

### Usage

gammaz(z)

122 gaussHermite

# **Arguments**

Z

Real or complex number or a numeric or complex vector.

#### **Details**

Computes the Gamma function for complex arguments using the Lanczos series approximation.

Accuracy is 15 significant digits along the real axis and 13 significant digits elsewhere.

To compute the logarithmic Gamma function use log(gammaz(z)).

#### Value

Returns a complex vector of function values.

#### Note

Copyright (c) 2001 Paul Godfrey for a Matlab version available on Mathwork's Matlab Central under BSD license.

Numerical Recipes used a 7 terms formula for a less effective approximation.

### References

Zhang, Sh., and J. Jin (1996). Computation of Special Functions. Wiley-Interscience, New York.

#### See Also

```
gamma, gsl::lngamma_complex
```

### **Examples**

```
max(gamma(1:10) - gammaz(1:10))
gammaz(-1)
gammaz(c(-2-2i, -1-1i, 0, 1+1i, 2+2i))

# Euler's reflection formula
z <- 1+1i
gammaz(1-z) * gammaz(z) # == pi/sin(pi*z)</pre>
```

gaussHermite

Gauss-Hermite Quadrature Formula

# Description

Nodes and weights for the n-point Gauss-Hermite quadrature formula.

# Usage

```
gaussHermite(n)
```

gaussHermite 123

### Arguments

n

Number of nodes in the interval ]-Inf, Inf[.

#### **Details**

Gauss-Hermite quadrature is used for integrating functions of the form

$$\int_{-\infty}^{\infty} f(x)e^{-x^2}dx$$

over the infinite interval  $]-\infty,\infty[$ .

x and w are obtained from a tridiagonal eigenvalue problem. The value of such an integral is then sum(w\*f(x)).

#### Value

List with components x, the nodes or points in]-Inf, Inf[, and w, the weights applied at these nodes.

#### Note

The basic quadrature rules are well known and can, e. g., be found in Gautschi (2004) — and explicit Matlab realizations in Trefethen (2000). These procedures have also been implemented in Matlab by Geert Van Damme, see his entries at MatlabCentral since 2010.

For other Matlab implementations of many quadrature rules see the web site <a href="http://people.sc.fsu.edu/~jburkardt/m\_src/m\_src.html">http://people.sc.fsu.edu/~jburkardt/m\_src/m\_src.html</a> by J. Burkardt, Florida State University.

### References

Gautschi, W. (2004). Orthogonal Polynomials: Computation and Approximation. Oxford University Press.

Trefethen, L. N. (2000). Spectral Methods in Matlab. SIAM, Society for Industrial and Applied Mathematics.

### See Also

gaussLegendre, gaussLaguerre

```
cc <- gaussHermite(17)
# Integrate exp(-x^2) from -Inf to Inf
sum(cc$w)  #=> 1.77245385090552 == sqrt(pi)
# Integrate x^2 exp(-x^2)
sum(cc$w * cc$x^2)  #=> 0.88622692545276 == sqrt(pi) /2
# Integrate cos(x) * exp(-x^2)
sum(cc$w * cos(cc$x))  #=> 1.38038844704314 == sqrt(pi)/exp(1)^0.25
```

124 gaussLaguerre

gaussLaguerre

Gauss-Laguerre Quadrature Formula

### **Description**

Nodes and weights for the n-point Gauss-Laguerre quadrature formula.

## Usage

```
gaussLaguerre(n, a = 0)
```

### Arguments

n Number of nodes in the interval [0, Inf[.

a exponent of x in the integrand: must be greater or equal to 0, otherwise the integral would not converge.

### **Details**

Gauss-Laguerre quadrature is used for integrating functions of the form

$$\int_0^\infty f(x)x^a e^{-x} dx$$

over the infinite interval  $]0, \infty[$ .

x and w are obtained from a tridiagonal eigenvalue problem. The value of such an integral is then sum(w\*f(x)).

### Value

List with components x, the nodes or points in [0, Inf [, and w, the weights applied at these nodes.

### Note

The basic quadrature rules are well known and can, e. g., be found in Gautschi (2004) — and explicit Matlab realizations in Trefethen (2000). These procedures have also been implemented in Matlab by Geert Van Damme, see his entries at MatlabCentral since 2010.

For other Matlab implementations of many quadrature rules see the web site <a href="http://people.sc.fsu.edu/~jburkardt/m\_src/m\_src.html">http://people.sc.fsu.edu/~jburkardt/m\_src/m\_src.html</a> by J. Burkardt, Florida State University.

#### References

Gautschi, W. (2004). Orthogonal Polynomials: Computation and Approximation. Oxford University Press.

Trefethen, L. N. (2000). Spectral Methods in Matlab. SIAM, Society for Industrial and Applied Mathematics.

gaussLegendre 125

### See Also

```
gaussLegendre, gaussHermite
```

### **Examples**

gaussLegendre

Gauss-Legendre Quadrature Formula

### **Description**

Nodes and weights for the n-point Gauss-Legendre quadrature formula.

### Usage

```
gaussLegendre(n, a, b)
```

# Arguments

- n Number of nodes in the interval [a,b].
- a, b lower and upper limit of the integral; must be finite.

#### **Details**

x and w are obtained from a tridiagonal eigenvalue problem.

### Value

List with components x, the nodes or points in[a,b], and w, the weights applied at these nodes.

#### Note

Gauss quadrature is not suitable for functions with singularities.

### References

Gautschi, W. (2004). Orthogonal Polynomials: Computation and Approximation. Oxford University Press.

Trefethen, L. N. (2000). Spectral Methods in Matlab. SIAM, Society for Industrial and Applied Mathematics.

126 gaussNewton

### See Also

gaussHermite, gaussLaguerre

### **Examples**

```
## Quadrature with Gauss-Legendre nodes and weights
f \leftarrow function(x) sin(x+cos(10*exp(x))/3)
#\dontrun{ezplot(f, -1, 1, fill = TRUE)}
cc <- gaussLegendre(51, -1, 1)</pre>
Q \leftarrow sum(cc$w * f(cc$x)) #=> 0.0325036515865218, true error: < 1e-15
# If f is not vectorized, do an explicit summation:
Q <- 0; x <- cc$x; w <- cc$w
for (i in 1:51) Q \leftarrow Q + w[i] * f(x[i])
# If f is infinite at b = 1, set b < -b - eps (with, e.g., eps = 1e-15)
# Use Gauss-Kronrod approach for error estimation
cc <- gaussLegendre(103, -1, 1)
abs(Q - sum(cc$w * f(cc$x)))
                                  # rel.error < 1e-10
# Use Gauss-Hermite for vector-valued functions
f \leftarrow function(x) c(sin(pi*x), exp(x), log(1+x))
cc <- gaussLegendre(32, 0, 1)
drop(cc$w %*% matrix(f(cc$x), ncol = 3)) # c(2/pi, exp(1) - 1, 2*log(2) - 1)
# absolute error < 1e-15
```

gaussNewton

Gauss-Newton Function Minimization

## **Description**

Gauss-Newton method of minimizing a term  $f_1(x)^2 + ... + f_m(x)^2$  or F'F where  $F = (f_1, ..., f_m)$  is a multivariate function of n variables, not necessarily n = m.

### Usage

```
gaussNewton(x0, Ffun, Jfun = NULL, maxiter = 100, tol = .Machine$double.eps^(1/2), ...)
```

## **Arguments**

Ffun m functions of n variables.

Jfun function returning the Jacobian matrix of Ffun; if NULL, the default, the Jacobian

will be computed numerically. The gradient of f will be computed internally

from the Jacobian (i.e., cannot be supplied).

x0 Numeric vector of length n.

maxiter Maximum number of iterations.

gaussNewton 127

tol Tolerance, relative accuracy.

... Additional parameters to be passed to f.

#### **Details**

Solves the system of equations applying the Gauss-Newton's method. It is especially designed for minimizing a sum-of-squares of functions and can be used to find a common zero of several function.

This algorithm is described in detail in the textbook by Antoniou and Lu, incl. different ways to modify and remedy the Hessian if not being positive definite. Here, the approach by Goldfeld, Quandt and Trotter is used, and the hessian modified by the Matthews and Davies algorithm if still not invertible.

To accelerate the iteration, an inexact linesearch is applied.

#### Value

List with components:

xs the minimum or root found so far,
fs the square root of sum of squares of the values of f,
iter the number of iterations needed, and
relerr the absoulte distance between the last two solutions.

### Note

If n=m then directly applying the newtonsys function might be a better alternative.

#### References

Antoniou, A., and W.-S. Lu (2007). Practical Optimization: Algorithms and Engineering Applications. Springer Business+Science, New York.

## See Also

```
newtonsys, softline
```

128 gauss\_kronrod

```
c(x[1]^2 + x[2]^2 - 2, exp(x[1] - 1) + x[2]^3 - 2)
gaussNewton(c(2.0, 0.5), f4)
# $xs
        1 1
## Examples (from Matlab)
F1 <- function(x) c(2*x[1]-x[2]-exp(-x[1]), -x[1]+2*x[2]-exp(-x[2]))
gaussNewton(c(-5, -5), F1)
# Find a matrix X such that X \%*% X \%*% X = [1 2; 3 4]
F2 <- function(x) {
    X \leftarrow matrix(x, 2, 2)
    D \leftarrow X \% \% X \% \% X - matrix(c(1,3,2,4), 2, 2)
    return(c(D))
sol <- gaussNewton(ones(2,2), F2)</pre>
(X <- matrix(sol$xs, 2, 2))</pre>
  [,1] [,2]
# [1,] -0.1291489 0.8602157
# [2,] 1.2903236 1.1611747
X %*% X %*% X
```

gauss\_kronrod

Gauss-Kronrod Quadrature

## **Description**

Simple Gaussian-Kronrod quadrature formula.

#### **Usage**

```
gauss_kronrod(f, a, b, ...)
```

### **Arguments**

f function to be integrated.

a, b end points of the interval.

... variables to be passed to the function.

### **Details**

Gaussian quadrature of degree 7 with Gauss-Kronrod of degree 15 for error estimation, the quadQK15 procedure in the QUADPACK library.

#### Value

List of value and relative error.

gcd, lcm

### Note

The function needs to be vectorized (though this could easily be changed), but the function does not need to be defined at the end points.

#### References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

#### See Also

```
quadgk, romberg
```

## **Examples**

gcd, 1cm

GCD and LCM Integer Functions

## **Description**

Greatest common divisor and least common multiple

## Usage

```
gcd(a, b, extended = FALSE)
Lcm(a, b)
```

## **Arguments**

a, b vectors of integers.

extended logical; if TRUE the extended Euclidean algorithm will be applied.

### **Details**

Computation based on the extended Euclidean algorithm.

If both a and b are vectors of the same length, the greatest common divisor/lowest common multiple will be computed elementwise. If one is a vektor, the other a scalar, the scalar will be replicated to the same length.

#### Value

A numeric (integer) value or vector of integers. Or a list of three vectors named c, d, g, g containing the greatest common divisors, such that

```
g = c * a + d * b.
```

geomean, harmmean

### Note

```
The following relation is always true:
```

```
n * m = gcd(n, m) * lcm(n, m)
```

#### See Also

```
numbers::extGCD
```

### **Examples**

```
gcd(12, 1:24) gcd(46368, 75025) # Fibonacci numbers are relatively prime to each other Lcm(12, 1:24) Lcm(46368, 75025) # = 46368 * 75025
```

geomean, harmmean

Geometric and Harmonic Mean (Matlab Style)

## **Description**

Geometric and harmonic mean along a dimension of a vector, matrix, or array. trimmean is almost the same as mean in R.

### Usage

```
geomean(x, dim = 1)
harmmean(x, dim = 1)
trimmean(x, percent = 0)
```

## **Arguments**

x numeric vector, matrix, or array.

dim dimension along which to take the mean; dim=1 means along columns, dim=2

along rows, the result will still be a row vector, not a column vector as in Matlab.

percent percentage, between 0 and 100, of trimmed values.

#### **Details**

trimmean does not call mean with the trim option, but rather calculates k<-round(n\*percent/100/2) and leaves out k values at the beginning and end of the sorted x vector (or row or column of a matrix).

### Value

Returns a scalar or vector (or array) of geometric or harmonic means: For dim=1 the mean of columns, dim=2 the mean of rows, etc.

geo\_median 131

#### Note

To have an exact analogue of mean(x) in Matlab, apply trimmean(x).

#### See Also

mean

### **Examples**

geo\_median

Geometric Median

### **Description**

Compute the "geometric median" of points in n-dimensional space, that is the point with the least sum of (Euclidean) distances to all these points.

## Usage

```
geo_median(P, tol = 1e-07, maxiter = 200)
```

## **Arguments**

P matrix of points, x\_i-coordinates in the ith column.

tol relative tolerance.

maxiter maximum number of iterations.

## Details

The task is solved applying an iterative process, known as Weiszfeld's algorithm. The solution is unique whenever the points are not collinear.

If the dimension is 1 (one column), the median will be returned.

### Value

Returns a list with components p the coordinates of the solution point, d the sum of distances to all the sample points, reltol the relative tolerance of the iterative process, and niter the number of iterations.

132 givens

## Note

This is also known as the "1-median problem" and can be generalized to the "k-median problem" for k cluster centers; see kcca in the 'flexclust' package.

### References

See Wikipedia's entry on "Geometric median".

#### See Also

```
L1linreg
```

## **Examples**

```
# Generate 100 points on the unit sphere in the 10-dim. space
set.seed(1001)
P <- rands(n=100, N=9)
( sol <- geo_median(P) )
# $p
# [1] -0.009481361 -0.007643410 -0.001252910  0.006437703 -0.019982885 -0.045337987
# [7]  0.036249563  0.003232175  0.035040592  0.046713023
# $d
# [1] 99.6638
# $reltol
# [1] 3.069063e-08
# $niter
# [1] 10</pre>
```

givens

Givens Rotation

### **Description**

Givens Rotations and QR decomposition

# Usage

```
givens(A)
```

### **Arguments**

Α

numeric square matrix.

## **Details**

```
givens(A) returns a QR decomposition (or factorization) of the square matrix A by applying unitary 2-by-2 matrices U such that U * [xk;xl] = [x,0] where x=sqrt(xk^2+xl^2)
```

gmres 133

## Value

List with two matrices Q and R, Q orthonormal and R upper triangular, such that A=Q%\*%R.

### References

Golub, G. H., and Ch. F. van Loan (1996). Matrix Computations. Third edition, John Hopkins University Press, Baltimore.

#### See Also

householder

## **Examples**

```
## QR decomposition
A <- matrix(c(0,-4,2, 6,-3,-2, 8,1,-1), 3, 3, byrow=TRUE)
gv <- givens(A)
(Q <- gv$Q); (R <- gv$R)
zapsmall(Q %*% R)
givens(magic(5))</pre>
```

gmres

Generalized Minimal Residual Method

# Description

gmres(A,b) attempts to solve the system of linear equations A\*x=b for x.

## Usage

```
gmres(A, b, x0 = rep(0, length(b)),
        errtol = 1e-6, kmax = length(b)+1, reorth = 1)
```

## **Arguments**

Α

	_
b	numerical vector or column vector.
x0	initial iterate.
errtol	relative residual reduction factor.
kmax	maximum number of iterations

square matrix.

reorth reorthogonalization method, see Details.

gmres gmres

### **Details**

Iterative method for the numerical solution of a system of linear equations. The method approximates the solution by the vector in a Krylov subspace with minimal residual. The Arnoldi iteration is used to find this vector.

Reorthogonalization method:

- 1 Brown/Hindmarsh condition (default)
- 2 Never reorthogonalize (not recommended)
- 3 Always reorthogonalize (not cheap!)

## Value

Returns a list with components x the solution, error the vector of residual norms, and niter the number of iterations.

### Author(s)

Based on Matlab code from C. T. Kelley's book, see references.

#### References

C. T. Kelley (1995). Iterative Methods for Linear and Nonlinear Equations. SIAM, Society for Industrial and Applied Mathematics, Philadelphia, USA.

## See Also

solve

```
A \leftarrow matrix(c(0.46, 0.60, 0.74, 0.61, 0.85,
              0.56, 0.31, 0.80, 0.94, 0.76,
              0.41, 0.19, 0.15, 0.33, 0.06,
              0.03, 0.92, 0.15, 0.56, 0.08,
              0.09, 0.06, 0.69, 0.42, 0.96), 5, 5)
x \leftarrow c(0.1, 0.3, 0.5, 0.7, 0.9)
b <- A %*% x
gmres(A, b)
# $x
       [,1]
# [1,] 0.1
# [2,] 0.3
# [3,] 0.5
# [4,] 0.7
# [5,] 0.9
# $error
# [1] 2.37446e+00 1.49173e-01 1.22147e-01 1.39901e-02 1.37817e-02 2.81713e-31
# $niter
# [1] 5
```

golden\_ratio 135

	golden_ratio	Golden Ratio Search
--	--------------	---------------------

# Description

Golden Ratio search for a univariate function minimum in a bounded interval.

# Usage

```
golden_ratio(f, a, b, ..., maxiter = 100, tol = .Machine$double.eps^0.5)
```

# Arguments

f	Function or its name as a string.
a, b	endpoints of the interval.
maxiter	maximum number of iterations.
tol	absolute tolerance; default sqrt(eps).
	Additional arguments to be passed to f.

### **Details**

'Golden ratio' search for a univariate function minimum in a bounded interval.

#### Value

Return a list with components xmin, fmin, the function value at the minimum, niter, the number of iterations done, and the estimated precision estim.prec

### See Also

uniroot

```
 f <- function(x) \ x \ * cos(0.1*exp(x)) \ * sin(0.1*pi*exp(x)) \\ golden_ratio(f, 0, 4, tol=10^-10) \ \# \ *xmin = 3.24848329206212 \\ optimize(f, c(0,4), tol=10^-10) \ \# \ *minimum = 3.24848328971188
```

136 grad

grad

Numerical Gradient

# Description

Numerical function gradient.

### Usage

```
grad(f, x0, heps = .Machine$double.eps^(1/3), ...)
```

### **Arguments**

f function of several variables.

x0 point where the gradient is to build.

heps step size.

... more variables to be passed to function f.

## **Details**

Computes the gradient

$$(\frac{\partial f}{\partial x_1}, \dots, \frac{\partial f}{\partial x_n})$$

numerically using the "central difference formula".

## Value

Vector of the same length as x0.

#### References

Mathews, J. H., and K. D. Fink (1999). Numerical Methods Using Matlab. Third Edition, Prentice Hall.

## See Also

fderiv

```
f <- function(u) {
    x <- u[1]; y <- u[2]; z <- u[3]
    return(x^3 + y^2 + z^2 +12*x*y + 2*z)
}
x0 <- c(1,1,1)
grad(f, x0)  # 15 14 4  # direction of steepest descent
sum(grad(f, x0) * c(1, -1, 0))  # 1 , directional derivative</pre>
```

gradient 137

```
f <- function(x) x[1]^2 + x[2]^2
grad(f, c(0,0)) # 0 0 , i.e. a local optimum
```

gradient

Discrete Gradient (Matlab Style)

### **Description**

Discrete numerical gradient.

## Usage

```
gradient(F, h1 = 1, h2 = 1)
```

## Arguments

F vector of function values, or a matrix of values of a function of two variables.

h1 x-coordinates of grid points, or one value for the difference between grid points in x-direction.

h2 y-coordinates of grid points, or one value for the difference between grid points in y-direction.

### Details

Returns the numerical gradient of a vector or matrix as a vector or matrix of discrete slopes in x-(i.e., the differences in horizontal direction) and slopes in y-direction (the differences in vertical direction).

A single spacing value, h, specifies the spacing between points in every direction, where the points are assumed equally spaced.

#### Value

If F is a vector, one gradient vector will be returned.

If F is a matrix, a list with two components will be returned:

X numerical gradient/slope in x-direction.
Y numerical gradient/slope in x-direction.

where each matrix is of the same size as F.

#### Note

TODO: If h2 is missing, it will not automatically be adapted.

### See Also

fderiv

138 gramSchmidt

### **Examples**

```
x < - seq(0, 1, by=0.2)
y \leftarrow c(1, 2, 3)
(M <- meshgrid(x, y))</pre>
gradient(M$X^2 + M$Y^2)
gradient(M$X^2 + M$Y^2, x, y)
## Not run:
# One-dimensional example
x \leftarrow seq(0, 2*pi, length.out = 100)
y < - \sin(x)
f <- gradient(y, x)</pre>
\max(f - \cos(x))
                      #=> 0.00067086
plot(x, y, type = "l", col = "blue")
lines(x, cos(x), col = "gray", lwd = 3)
lines(x, f, col = "red")
grid()
# Two-dimensional example
v \leftarrow seq(-2, 2, by=0.2)
X <- meshgrid(v, v)$X</pre>
Y <- meshgrid(v, v)$Y
Z <- X * exp(-X^2 - Y^2)
image(v, v, t(Z))
contour(v, v, t(Z), col="black", add = TRUE)
grid(col="white")
grX <- gradient(Z, v, v)$X</pre>
grY <- gradient(Z, v, v)$Y</pre>
quiver(X, Y, grX, grY, scale = 0.2, col="blue")
## End(Not run)
```

gramSchmidt

Gram-Schmidt

### **Description**

Modified Gram-Schmidt Process

### Usage

```
gramSchmidt(A, tol = .Machine$double.eps^0.5)
```

### **Arguments**

A numeric matrix with nrow(A)>=ncol(A).
tol numerical tolerance for being equal to zero.

hadamard 139

### **Details**

The modified Gram-Schmidt process uses the classical orthogonalization process to generate step by step an orthonoral basis of a vector space. The modified Gram-Schmidt iteration uses orthogonal projectors in order ro make the process numerically more stable.

#### Value

List with two matrices Q and R, Q orthonormal and R upper triangular, such that A=Q%\*%R.

#### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Society for Industrial and Applied Mathematics, Philadelphia.

### See Also

```
householder, givens
```

## **Examples**

```
## QR decomposition A <- matrix(c(0,-4,2,6,-3,-2,8,1,-1), 3, 3, byrow=TRUE) gs <- gramSchmidt(A) (Q <- gs$Q); (R <- gs$R) Q %*% R # = A
```

hadamard

Hadamard Matrix

### **Description**

Generate Hadamard matrix of a certain size.

### Usage

hadamard(n)

### **Arguments**

n

An integer of the form 2<sup>e</sup>, 12\*2<sup>e</sup>, or 20\*2<sup>e</sup>

### **Details**

An n-by-n Hadamard matrix with n>2 exists only if rem(n,4)=0. This function handles only the cases where n, n/12, or n/20 is a power of 2.

### Value

Matrix of size n-by-n of orthogonal columns consisting of 1 and -1 only.

140 halley

## Note

Hadamard matrices have applications in combinatorics, signal processing, and numerical analysis.

#### See Also

```
hankel, Toeplitz
```

## **Examples**

```
hadamard(4)
H <- hadamard(8)
t(H)</pre>
```

halley

Halley's Root Finding Mathod

# **Description**

Finding roots of univariate functions using the Halley method.

### Usage

```
halley(fun, x0,
maxiter = 100, tol = .Machine$double.eps^0.5)
```

## Arguments

fun function whose root is to be found.

x0 starting value for the iteration.

maxiter maximum number of iterations.

tol absolute tolerance; default eps^(1/2)

## **Details**

Well known root finding algorithms for real, univariate, continuous functions; the second derivative must be smooth, i.e. continuous. The first and second derivative are computed numerically.

#### Value

Return a list with components root, f.root, the function value at the found root, iter, the number of iterations done, and the estimated precision estim.prec

### References

http://mathworld.wolfram.com/HalleysMethod.html

hampel 141

### See Also

newtonRaphson

# **Examples**

```
halley(sin, 3.0)  # 3.14159265358979 in the 3 iterations halley(function(x) x*exp(x) - 1, 1.0)  # 0.567143290409784 Gauss' omega constant  # Legendre polynomial of degree 5 lp5 <- c(63, 0, -70, 0, 15, 0)/8  f <- function(x) polyval(lp5, x)  halley(f, 1.0)  # 0.906179845938664
```

hampel

Hampel Filter

### **Description**

Median absolute deviation (MAD) outlier in Time Series

### Usage

```
hampel(x, k, t0 = 3)
```

### **Arguments**

x numeric vector representing a time series

k window length 2\*k+1 in indices

threshold, default is 3 (Pearson's rule), see below.

## **Details**

The 'median absolute deviation' computation is done in the [-k...k] vicinity of each point at least k steps away from the end points of the interval. At the lower and upper end the time series values are preserved.

A high threshold makes the filter more forgiving, a low one will declare more points to be outliers. t0<-3 (the default) corresponds to Ron Pearson's 3 sigma edit rule, t0<-0 to John Tukey's median filter.

#### Value

Returning a list L with L\$y the corrected time series and L\$ind the indices of outliers in the 'median absolut deviation' sense.

142 hankel

## Note

Don't take the expression *outlier* too serious. It's just a hint to values in the time series that appear to be unusual in the vicinity of their neighbors under a normal distribution assumption.

### References

Pearson, R. K. (1999). "Data cleaning for dynamic modeling and control". European Control Conference, ETH Zurich, Switzerland.

### See Also

findpeaks

## **Examples**

```
set.seed(8421)
x <- numeric(1024)
z <- rnorm(1024)
x[1] <- z[1]
for (i in 2:1024) {
x[i] <- 0.4*x[i-1] + 0.8*x[i-1]*z[i-1] + z[i]
}
omad <- hampel(x, k=20)

## Not run:
plot(1:1024, x, type="1")
points(omad$ind, x[omad$ind], pch=21, col="darkred")
grid()
## End(Not run)</pre>
```

hankel

Hankel Matrix

# Description

Generate Hankel matrix from column and row vector

## Usage

```
hankel(a, b)
```

## **Arguments**

- a vector that will be the first column
- b vector that if present will form the last row.

hausdorff\_dist 143

### **Details**

hankel(a) returns the square Hankel matrix whose first column is a and whose elements are zero below the secondary diagonal. (I.e.: b may be missing.)

hankel(a, b) returns a Hankel matrix whose first column is a and whose last row is b. If the first element of b differs from the last element of a it is overwritten by this one.

### Value

```
matrix of size (length(a), length(b))
```

#### See Also

```
Toeplitz, hadamard
```

### **Examples**

```
hankel(1:5, 5:1)
```

hausdorff\_dist

Hausdorff Distance

## Description

Hausdorff distance (aka Hausdorff dimension)

#### Usage

```
hausdorff_dist(P, Q)
```

# **Arguments**

P, Q

numerical matrices, representing points in an m-dim. space.

#### **Details**

Calculates the Hausdorff Distance between two sets of points, P and Q. Sets P and Q must be matrices with the same number of columns (dimensions).

The 'directional' Hausdorff distance (dhd) is defined as:

```
dhd(P,Q) = max p in P [min q in Q [||p-q||]]
```

Intuitively dhd finds the point p from the set P that is farthest from any point in Q and measures the distance from p to its nearest neighbor in Q. The Hausdorff Distance is defined as max(dhd(P,Q),dhd(Q,P)).

### Value

A single scalar, the Hausdorff distance (dimension).

144 hessian

### References

Barnsley, M. (1993). Fractals Everywhere. Morgan Kaufmann, San Francisco.

#### See Also

```
distmat
```

## **Examples**

hessian

Hessian Matrix

# **Description**

Numerically compute the Hessian matrix.

## Usage

```
hessian(f, x0, h = .Machine$double.eps^(1/4), ...)
```

## **Arguments**

f univariate function of several variables.

x0 point in  $\mathbb{R}^n$ .

... variables to be passed to f.

#### **Details**

Computes the hessian matrix based on the three-point central difference formula, expanded to two variables.

Assumes that the function has continuous partial derivatives.

### Value

```
An n-by-n matrix with \frac{\partial^2 f}{\partial x_i \partial x_j} as (i, j) entry.
```

# References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

hilb 145

## See Also

```
laplacian
```

# **Examples**

```
f <- function(x) cos(x[1] + x[2])
x0 <- c(0, 0)
hessian(f, x0)

f <- function(u) {
    x <- u[1]; y <- u[2]; z <- u[3]
    return(x^3 + y^2 + z^2 +12*x*y + 2*z)
}
x0 <- c(1,1,1)
hessian(f, x0)</pre>
```

hilb

Hilbert Matrix

## **Description**

Generate Hilbert matrix of dimension n

# Usage

hilb(n)

# Arguments

n

positive integer specifying the dimension of the Hilbert matrix

## **Details**

```
Generate the Hilbert matrix H of dimension n with elements H[i, j] = 1/(i+j-1). (Note: This matrix is ill-conditioned, see e.g. det(hilb(6)).)
```

### Value

matrix of dimension n

### See Also

vander

# **Examples**

hilb(5)

146 histe

histc

Histogram Count (Matlab style)

### **Description**

Histogram-like counting.

## Usage

```
histc(x, edges)
```

### **Arguments**

x numeric vector or matrix.

edges numeric vector of grid points, must be monotonically non-decreasing.

#### **Details**

n = histc(x,edges) counts the number of values in vector x that fall between the elements in the edges vector (which must contain monotonically nondecreasing values). n is a length(edges) vector containing these counts.

If x is a matrix then cnt and bin are matrices too, and

```
for (j in (1:n)) cnt[k,j] \leftarrow sum(bin[, j] == k)
```

### Value

returns a list with components cnt and bin. n(k) counts the number of values in x that lie between edges(k) <= x(i) < edges(k+1). The last counts any values of x that match edges(n). Values outside the values in edges are not counted. Use -Inf and Inf in edges to include all values.

```
bin[i] returns k if edges(k) \leq x(i) \leq edges(k+1), and 0 if x[i] lies outside the grid.
```

#### See Also

hist, codehistss, findInterval

```
x <- seq(0.0, 1.0, by = 0.05)
e <- seq(0.1, 0.9, by = 0.10)
histc(x, e)
# $cnt
# [1] 2 2 2 2 2 2 2 2 2 1
# $bin
# [1] 0 0 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 0 0
## Not run:
# Compare</pre>
```

histss 147

```
findInterval(x, e)
# [1] 0 0 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9 9
findInterval(x, e, all.inside = TRUE)
# [1] 1 1 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 8 8 8
# cnt[i] <- sum(findInterval(x, e) == i)</pre>
## End(Not run)
x \leftarrow matrix(c(0.5029, 0.2375, 0.2243, 0.8495,
             0.0532, 0.1644, 0.4215, 0.4135,
             0.7854, 0.0879, 0.1221, 0.6170), 3, 4, byrow = TRUE)
e < - seq(0.0, 1.0, by = 0.2)
histc(x, e)
# $cnt
      [,1] [,2] [,3] [,4]
# [1,]
            2 1
        1
# [2,]
         0
             1
                  1
                1
# [3,]
        1 0
                       1
       1 0 0
# [4,]
                     1
       0 0 0 1
# [5,]
# [6,]
# $bin
      [,1] [,2] [,3] [,4]
# [1,]
       3 2 2
        1 1
# [2,]
                  3
                       3
                1
# [3,]
             1
         4
                       4
```

histss

Histogram Bin-width Optimization

# Description

Method for selecting the bin size of time histograms.

## Usage

```
histss(x, n = 100, plotting = FALSE)
```

## Arguments

x numeric vector or matrix.n maximum number of bins.plotting logical; shall a histogram be plotted.

### **Details**

Bin sizes of histograms are optimized in a way to best displays the underlying spike rate, for example in neurophysiological studies.

hooke\_jeeves

## Value

Returns the same list as the hist function; the list is invisible if the histogram is plotted.

### References

Shimazaki H. and S. Shinomoto. A method for selecting the bin size of a time histogram. Neural Computation (2007) Vol. 19(6), 1503-1527

#### See Also

```
hist, histc
```

## **Examples**

```
x <- sin(seq(0, pi/2, length.out = 200))
H <- histss(x, n = 50, plotting = FALSE)
## Not run:
plot(H, col = "gainsboro") # Compare with hist(x), or
hist(x, breaks = H$breaks) # the same
## End(Not run)</pre>
```

hooke\_jeeves

Hooke-Jeeves Minimization Method

# Description

An implementation of the Hooke-Jeeves algorithm for derivative-free optimization.

## Usage

```
hooke_jeeves(x0, f, lb = NULL, ub = NULL, tol = 1e-08,
target = Inf, maxfeval = Inf, info = FALSE, ...)
```

## **Arguments**

x0	starting vector.
f	nonlinear function to be minimized.
lb, ub	lower and upper bounds.
tol	relative tolerance, to be used as stopping rule.
target	iteration stops when this value is reached.
maxfeval	maximum number of allowed function evaluations.
info	logical, whether to print information during the main loop.
	additional arguments to be passed to the function.

hooke\_jeeves 149

### **Details**

This method computes a new point using the values of f at suitable points along the orthogonal coordinate directions around the last point.

### Value

List with following components:

xmin minimum solution found so far.fmin value of f at minimum.fcalls number of function evaluations.niter number of iterations performed.

#### Note

Hooke-Jeeves is notorious for its number of function calls. Memoization is often suggested as a remedy.

For a similar implementation of Hooke-Jeeves see the 'dfoptim' package.

#### References

```
C.T. Kelley (1999), Iterative Methods for Optimization, SIAM.
Quarteroni, Sacco, and Saleri (2007), Numerical Mathematics, Springer.
```

### See Also

```
nelder_mead
```

```
## Rosenbrock function
rosenbrock <- function(x) {</pre>
    n \leftarrow length(x)
    x1 <- x[2:n]
    x2 <- x[1:(n-1)]
    sum(100*(x1-x2^2)^2 + (1-x2)^2)
}
hooke\_jeeves(c(0,0,0,0), rosenbrock)
# $xmin
# [1] 1.000000 1.000001 1.000002 1.000004
# $fmin
# [1] 4.774847e-12
# $fcalls
# [1] 2499
# $niter
#[1] 26
hooke_jeeves(rep(0,4), lb=rep(-1,4), ub=0.5, rosenbrock)
```

horner

```
# $xmin
# [1] 0.50000000 0.26221320 0.07797602 0.00608027
# $fmin
# [1] 1.667875
# $fcalls
# [1] 571
# $niter
# [1] 26
```

horner

Horner's Rule

### **Description**

Compute the value of a polynomial via Horner's Rule.

### Usage

```
horner(p, x)
hornerdefl(p, x)
```

# Arguments

p Numeric vector representing a polynomial.

x Numeric scalar, vector or matrix at which to evaluate the polynomial.

## **Details**

horner utilizes the Horner scheme to evaluate the polynomial and its first derivative at the same time.

The polynomial  $p = p_1*x^n + p_2*x^{n-1} + ... + p_n*x + p_{n+1}$  is hereby represented by the vector  $p_1, p_2, ..., p_n, p_{n+1}$ , i.e. from highest to lowest coefficient.

hornerdefl uses a similar approach to return the value of p at x and a polynomial q that satisfies

```
p(t) = q(t) * (t - x) + r, r constant
```

which implies r=0 if x is a root of p. This will allow for a repeated root finding of polynomials.

#### Value

horner returns a list with two elements, list(y=..., dy=...) where the first list elements returns the values of the polynomial, the second the values of its derivative at the point(s) x.

hornerdefl returns a list list(y=..., dy=...) where q represents a polynomial, see above.

#### Note

For fast evaluation, there is no error checking for p and x, which both must be numerical vectors (x can be a matrix in horner).

householder 151

### References

Quarteroni, A., and Saleri, F. (2006) Scientific Computing with Matlab and Octave. Second Edition, Springer-Verlag, Berlin Heidelberg.

## See Also

```
polyval
```

## **Examples**

```
x \leftarrow c(-2, -1, 0, 1, 2)

p \leftarrow c(1, 0, 1) # polynomial x^2 + x, derivative 2*x

horner(p, x)$y #=> 5 2 1 2 5

horner(p, x)$dy #=> -4 -2 0 2 4

p \leftarrow Poly(c(1, 2, 3)) # roots 1, 2, 3

hornerdefl(p, 3) # q = x^2 - 3 x + 2 with roots 1, 2
```

householder

Householder Reflections

### **Description**

Householder reflections and QR decomposition

## Usage

householder(A)

## **Arguments**

Α

numeric matrix with nrow(A)>=ncol(A).

#### **Details**

The Householder method applies a succession of elementary unitary matrices to the left of matrix A. These matrices are the so-called Householder reflections.

# Value

List with two matrices Q and R, Q orthonormal and R upper triangular, such that A=Q%\*%R.

### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Society for Industrial and Applied Mathematics, Philadelphia.

humps

### See Also

givens

## **Examples**

```
## QR decomposition
A <- matrix(c(0,-4,2,6,-3,-2,8,1,-1), 3, 3, byrow=TRUE)
S <- householder(A)</pre>
(Q <- S$Q); (R <- S$R)
Q \% * R # = A
## Solve an overdetermined linear system of equations
A \leftarrow matrix(c(1:8,7,4,2,3,4,2,2), ncol=3, byrow=TRUE)
S \leftarrow householder(A); Q \leftarrow S$Q; R \leftarrow S$R
m <- nrow(A); n <- ncol(A)</pre>
b < -rep(6, 5)
x <- numeric(n)</pre>
b <- t(Q) %*% b
x[n] \leftarrow b[n] / R[n, n]
for (k in (n-1):1)
    x[k] \leftarrow (b[k] - R[k, (k+1):n] %*% x[(k+1):n]) / R[k, k]
qr.solve(A, rep(6, 5)); x
```

humps

Matlab Test Functions

## **Description**

Matlab test functions.

## Usage

```
humps(x)
sinc(x)
```

## Arguments

Х

Numeric scalar or vector.

#### **Details**

humps is a test function for finding zeros, for optimization and integration. Its root is at x = 1.2995, a (local) minimum at x = 0.6370, and the integral from 0.5 to 1.0 is 8.0715.

sinc is defined as  $sinc(t) = \frac{\sin(\pi t)}{\pi t}$ . It is the continuous inverse Fourier transform of the rectangular pulse of width  $2\pi$  and height 1.

hurstexp 153

### Value

Numeric scalar or vector.

# Examples

```
## Not run:
plot(humps(), type="l"); grid()

x <- seq(0, 10, length=101)
plot(x, sinc(x), type="l"); grid()
## End(Not run)</pre>
```

hurstexp

Hurst Exponent

# Description

Calculates the Hurst exponent using R/S analysis.

# Usage

```
hurstexp(x, d = 50, display = TRUE)
```

### **Arguments**

x a time series.

d smallest box size; default 50.

display logical; shall the results be printed to the console?

## **Details**

hurstexp(x) calculates the Hurst exponent of a time series x using R/S analysis, after Hurst, with slightly different approaches, or corrects it with small sample bias, see for example Weron.

These approaches are a corrected R/S method, an empirical and corrected empirical method, and a try at a theoretical Hurst exponent. It should be mentioned that the results are sometimes very different, so providing error estimates will be highly questionable.

Optimal sample sizes are automatically computed with a length that possesses the most divisors among series shorter than x by no more than 1 percent.

154 hurstexp

#### Value

hurstexp(x) returns a list with the following components:

- Hs simplified R over S approach
- Hrs corrected R over S Hurst exponent
- He empirical Hurst exponent
- Hal corrected empirical Hurst exponent
- Ht theoretical Hurst exponent

### Note

Derived from Matlab code of R. Weron, published on Matlab Central.

#### References

H.E. Hurst (1951) Long-term storage capacity of reservoirs, Transactions of the American Society of Civil Engineers 116, 770-808.

R. Weron (2002) Estimating long range dependence: finite sample properties and confidence intervals, Physica A 312, 285-299.

#### See Also

```
fractal::hurstSpec, RoverS, hurstBlock and fArma::LrdModelling
```

```
## Computing the Hurst exponent
data(brown72)
x72 <- brown72
                                       # H = 0.72
                                       # H = 0.50
xgn <- rnorm(1024)
xlm \leftarrow numeric(1024); xlm[1] \leftarrow 0.1  # H = 0.43
for (i in 2:1024) xlm[i] \leftarrow 4 * xlm[i-1] * (1 - xlm[i-1])
\begin{array}{lll} hurstexp(brown72, \ d = 128) & \# \ 0.72 \\ \# \ Simple \ R/S \ Hurst \ estimation: & 0.6590931 \end{array}
# Corrected R over S Hurst exponent: 0.7384611
# Empirical Hurst exponent: 0.7068613
# Corrected empirical Hurst exponent: 0.6838251
# Theoretical Hurst exponent: 0.5294909
# Corrected R over S Hurst exponent: 0.5982146
# Empirical Hurst exponent:
                                      0.6104621
# Corrected empirical Hurst exponent: 0.5690305
# Theoretical Hurst exponent:
                                      0.5368124
hurstexp(xlm)
                                    # 0.43
# Simple R/S Hurst estimation: 0.4825898
# Corrected R over S Hurst exponent: 0.5067766
```

hypot 155

```
# Empirical Hurst exponent:
                                       0.4869625
# Corrected empirical Hurst exponent: 0.4485892
# Theoretical Hurst exponent:
                                       0.5368124
## Compare with other implementations
## Not run:
library(fractal)
x <- x72
hurstSpec(x)
                                # 0.776
                                          # 0.720
RoverS(x)
                                # 0.717
hurstBlock(x, method="aggAbs") # 0.648
hurstBlock(x, method="aggVar") # 0.613
hurstBlock(x, method="diffvar") # 0.714
hurstBlock(x, method="higuchi") # 1.001
x <- xgn
hurstSpec(x)
                                # 0.538
                                          # 0.500
RoverS(x)
                                # 0.663
hurstBlock(x, method="aggAbs") # 0.463
hurstBlock(x, method="aggVar") # 0.430
hurstBlock(x, method="diffvar") # 0.471
hurstBlock(x, method="higuchi") # 0.574
x \leftarrow x1m
hurstSpec(x)
                                # 0.478
                                          # 0.430
RoverS(x)
                                # 0.622
hurstBlock(x, method="aggAbs") # 0.316
hurstBlock(x, method="aggVar") # 0.279
hurstBlock(x, method="diffvar") # 0.547
hurstBlock(x, method="higuchi") # 0.998
## End(Not run)
```

hypot

Hypotenuse Function

# Description

Square root of sum of squares

## Usage

```
hypot(x, y)
```

### **Arguments**

x, y Vectors of real or complex numbers of the same size

156 ifft

## **Details**

Element-by-element computation of the square root of the sum of squares of vectors resp. matrices x and v.

### Value

Returns a vector or matrix of the same size.

### Note

Returns c() if x or y is empty and the other one has length 1. In all other cases, x and y have to be of the same size.

# **Examples**

```
hypot(3,4)
hypot(c(0, 0), c(3, 4))
```

ifft

Inverse Fast Fourier Transformation

## **Description**

Performs the inverse Fast Fourier Transform.

## Usage

```
ifft(x)
ifftshift(x)
fftshift(x)
```

## **Arguments**

Χ

a real or complex vector

## **Details**

ifft returns the value of the normalized discrete, univariate, inverse Fast Fourier Transform of the values in x.

ifftshift and fftshift shift the zero-component to the center of the spectrum, that is swap the left and right half of x.

## Value

Real or complex vector of the same length.

inpolygon 157

## Note

Almost an alias for R's fft(x, inverse=TRUE), but dividing by length(x).

#### See Also

fft

## **Examples**

```
x \leftarrow c(1, 2, 3, 4)
(y <- fft(x))
ifft(x)
ifft(y)
## Compute the derivative: F(df/dt) = (1i*k) * F(f)
   hyperbolic secans f <- sech
df \leftarrow function(x) - sech(x) * tanh(x)
d2f \leftarrow function(x) sech(x) - 2*sech(x)^3
L <- 20
                                            # domain [-L/2, L/2]
N <- 128
                                            # number of Fourier nodes
x \leftarrow linspace(-L/2, L/2, N+1)
                                            # domain discretization
x \leftarrow x[1:N]
                                            # because of periodicity
dx <- x[2] - x[1]
                                            # finite difference
u \leftarrow sech(x)
                                            # hyperbolic secans
u1d \leftarrow df(x); u2d \leftarrow d2f(x)
                                            # first and second derivative
                                            # discrete Fourier transform
ut <- fft(u)
k \leftarrow (2*pi/L)*fftshift((-N/2):(N/2-1)) # shifted frequencies
u1 <- Re(ifft((1i*k) * ut))
                                           # inverse transform
u2 \leftarrow Re(ifft(-k^2 * ut))
                                           # first and second derivative
## Not run:
plot(x, u1d, type = "1", col = "blue")
points(x, u1)
grid()
figure()
plot(x, u2d, type = "1", col = "darkred")
points(x, u2)
grid()
## End(Not run)
```

inpolygon

Polygon Region

# Description

Points inside polygon region.

### Usage

```
inpolygon(x, y, xp, yp, boundary = FALSE)
```

inpolygon inpolygon

# Arguments

x, y	x-, y-coordinates of points to be tested for being inside the polygon region.
xp, yp	coordinates of the vertices specifying the polygon.
boundary	Logical; does the boundary belong to the interior.

### **Details**

For a polygon defined by points (xp, yp), determine if the points (x, y) are inside or outside the polygon. The boundary can be included or excluded (default) for the interior.

#### Value

Logical vector, the same length as x.

#### Note

Special care taken for points on the boundary.

#### References

Hormann, K., and A. Agathos (2001). The Point in Polygon Problem for Arbitrary Polygons. Computational Geometry, Vol. 20, No. 3, pp. 131–144.

### See Also

polygon

```
xp \leftarrow c(0.5, 0.75, 0.75, 0.5, 0.5)
yp \leftarrow c(0.5, 0.5, 0.75, 0.75, 0.5)
x \leftarrow c(0.6, 0.75, 0.6, 0.5)
y < -c(0.5, 0.6, 0.75, 0.6)
inpolygon(x, y, xp, yp, boundary = FALSE) # FALSE
inpolygon(x, y, xp, yp, boundary = TRUE) # TRUE
## Not run:
pg \leftarrow matrix(c(0.15, 0.75, 0.25, 0.45, 0.70,
                0.80, 0.35, 0.55, 0.20, 0.90), 5, 2)
plot(c(0, 1), c(0, 1), type="n")
polygon(pg[,1], pg[,2])
P <- matrix(runif(20000), 10000, 2)
R <- inpolygon(P[, 1], P[, 2], pg[, 1], pg[,2])</pre>
clrs <- ifelse(R, "red", "blue")</pre>
points(P[, 1], P[, 2], pch = ".", col = clrs)
## End(Not run)
```

integral 159

### **Description**

Combines several approaches to adaptive numerical integration of functions of one variable.

## Usage

### **Arguments**

fun integrand, univariate (vectorized) function.

xmin, xmax endpoints of the integration interval.

method integration procedure, see below.

vectorized logical; is the integrand a vectorized function; not used.

arrayValued logical; is the integrand array-valued.

reltol relative tolerance.

abstol absolute tolerance; not used.

... additional parameters to be passed to the function.

### **Details**

integral combines the following methods for adaptive numerical integration (also available as separate functions):

- Kronrod (Gauss-Kronrod)
- Richardson (Gauss-Richardson)
- Clenshaw (Clenshaw-Curtis; not yet made adaptive)
- Simpson (adaptive Simpson)
- Romberg

Recommended default method is Gauss-Kronrod. Most methods require that function f is vectorized.

If the interval is infinite, quadinf will be called that accepts the same methods as well. If the function is array-valued, quadv is called that applies an adaptive Simpson procedure – other methods are ignored.

#### Value

Returns the integral, no error terms given.

160 integral

#### Note

integral does not provide 'new' functionality, everything is already contained in the functions called here.

#### References

Davis, Ph. J., and Ph. Rabinowitz (1984). Methods of Numerical Integration. Dover Publications, New York.

#### See Also

quadgk, quadgr, quadcc, simpadpt, romberg, quadv, quadinf

```
## Very smooth function
fun <- function(x) 1/(x^4+x^2+0.9)
val <- 1.582232963729353
for (m in c("Kron", "Rich", "Clen", "Simp", "Romb")) {
    Q \leftarrow integral(fun, -1, 1, reltol = 1e-12, method = m)
    cat(m, Q, abs(Q-val), "\n")
# Kron 1.582233 3.197442e-13
# Rich 1.582233 3.197442e-13
# Clen 1.582233 3.199663e-13
# Simp 1.582233 3.241851e-13
# Romb 1.582233 2.555733e-13
## Highly oscillating function
fun <- function(x) sin(100*pi*x)/(pi*x)</pre>
val <- 0.4989868086930458
for (m in c("Kron", "Rich", "Clen", "Simp", "Romb")) {
    Q <- integral(fun, 0, 1, reltol = 1e-12, method = m)
    cat(m, Q, abs(Q-val), "\n")}
# Kron 0.4989868 2.775558e-16
# Rich 0.4989868 4.440892e-16
# Clen 0.4989868 2.231548e-14
# Simp 0.4989868 6.328271e-15
# Romb 0.4989868 1.508793e-13
## Evaluate improper integral
fun <- function(x) log(x)^2 * exp(-x^2)
val <- 1.9475221803007815976
for (m in c("Kron", "Rich", "Clen", "Simp", "Romb")) {
    Q <- integral(fun, 0, Inf, reltol = 1e-12, method = m)
    cat(m, Q, abs(Q-val), "\n")
# Kron 1.947522 1.101341e-13
# Rich 1.947522 2.928655e-10
# Clen 1.948016 1.960654e-13
# Simp 1.947522 9.416912e-12
# Romb 1.952683 0.00516102
## Array-valued function
```

integral2 161

```
\begin{aligned} &\log 1 <- \; \text{function}(x) \; \log (1+x) \\ &\text{fun} <- \; \text{function}(x) \; \text{c}(\exp(x), \; \log 1(x)) \\ &\text{Q} <- \; \text{integral}(\text{fun}, \; 0, \; 1, \; \text{reltol} \; = \; 1e-12, \; \text{arrayValued} \; = \; \text{TRUE}, \; \text{method} \; = \; \text{"Simpson"}) \\ &\text{abs}(Q \; - \; \text{c}(\exp(1)-1, \; \log(4)-1)) & \# \; 2.220446e-16 \; 4.607426e-15 \end{aligned}
```

integral2

Numerically Evaluate Double and Triple Integrals

## **Description**

Numerically evaluate a double integral, resp. a triple integral by reducing it to a double integral.

### Usage

## **Arguments**

fun	function
xmin, xmax	lower and upper limits of x.
ymin, ymax	lower and upper limits of y.
zmin, zmax	lower and upper limits of z.
sector	logical.
reltol	relative tolerance.
abstol	absolute tolerance.
maxlist	maximum length of the list of rectangles.
singular	logical; are there singularities at vertices.
vectorized	logical; is the function fully vectorized.
	additional parameters to be passed to the function.

### **Details**

integral 2 implements the 'TwoD' algorithm, that is Gauss-Kronrod with (3, 7)-nodes on 2D rectangles.

The borders of the domain of integration must be finite. The limits of y, that is ymin and ymax, can be constants or scalar functions of x that describe the lower and upper boundaries. These functions must be vectorized.

integral 2 attempts to satisfy ERRBND  $\leq \max(AbsTol,RelTol*|Q|)$ . This is absolute error control when |Q| is sufficiently small and relative error control when |Q| is larger.

integral2

The function fun itself must be fully vectorized: It must accept arrays X and Y and return an array Z = f(X,Y) of corresponding values. If option vectorized is set to FALSE the procedure will enforce this vectorized behavior.

With sector=TRUE the region is a generalized sector that is described in polar coordinates (r,theta) by

```
0 \le a \le b - a and b must be constants c \le r \le d - c and d can be constants or ...
```

... functions of theta that describe the lower and upper boundaries. Functions must be vectorized. NOTE Polar coordinates are used only to describe the region – the integrand is f(x,y) for both kinds of regions.

integral2 can be applied to functions that are singular on a boundary. With value singular=TRUE, this option causes integral2 to use transformations to weaken singularities for better performance.

integral 3 also accepts functions for the inner interval limits. ymin, ymax must be constants or functions of one variable (x), zmin, zmax constants or functions of two variables (x, y), all functions vectorized.

The triple integral will be first integrated over the second and third variable with integral2, and then integrated over a single variable with integral.

#### Value

Returns a list with Q the integral and error the error term.

### Note

To avoid recursion, a possibly large matrix will be used and passed between subprograms. A more efficient implementation may be possible.

### Author(s)

Copyright (c) 2008 Lawrence F. Shampine for Matlab code and description of the program; adapted and converted to R by Hans W Borchers.

## References

Shampine, L. F. (2008). MATLAB Program for Quadrature in 2D. Proceedings of Applied Mathematics and Computation, 2008, pp. 266–274.

#### See Also

```
integral, cubature:adaptIntegrate
```

```
fun <- function(x, y) cos(x) * cos(y)
integral2(fun, 0, 1, 0, 1, reltol = 1e-10)
# $Q:     0.708073418273571 # 0.70807341827357119350 = sin(1)^2
# $error: 8.618277e-19 # 1.110223e-16</pre>
```

interp1 163

```
## Compute the volume of a sphere
f \leftarrow function(x, y) sqrt(1 - x^2 - y^2)
xmin <- 0; xmax <- 1</pre>
ymin <- 0; ymax <- function(x) sqrt(1 - x^2)
I <- integral2(f, xmin, xmax, ymin, ymax)</pre>
                                   # 0.5236076 - pi/6 => 8.800354e-06
## Compute the volume over a sector
I <- integral2(f, 0,pi/2, 0,1, sector = TRUE)</pre>
                                   # 0.5236308 - pi/6 => 3.203768e-05
## Integrate 1/( \operatorname{sqrt}(x + y)*(1 + x + y)^2 ) over the triangle
## 0 \le x \le 1, 0 \le y \le 1 - x. The integrand is infinite at (0,0).
f \leftarrow function(x,y) 1/( sqrt(x + y) * (1 + x + y)^2 )
ymax < - function(x) 1 - x
I <- integral2(f, 0,1, 0,ymax)</pre>
I$Q + 1/2 - pi/4
                                   # -3.247091e-08
## Compute this integral as a sector
rmax <- function(theta) 1/(sin(theta) + cos(theta))</pre>
I <- integral2(f, 0,pi/2, 0,rmax, sector = TRUE, singular = TRUE)</pre>
I$Q + 1/2 - pi/4
                                   # -4.998646e-11
## Examples of computing triple integrals
f0 \leftarrow function(x, y, z) y*sin(x) + z*cos(x)
integral3(f0, 0, pi, 0,1, -1,1) # - 2.0 => 0.0
f1 \leftarrow function(x, y, z) exp(x+y+z)
integral3(f1, 0, 1, 1, 2, 0, 0.5)
## [1] 5.206447
                                            # 5.20644655
f2 \leftarrow function(x, y, z) x^2 + y^2 + z
a <- 2; b <- 4
ymin \leftarrow function(x) x - 1
ymax <- function(x) x + 6
zmin <- -2
zmax \leftarrow function(x, y) 4 + y^2
integral3(f2, a, b, ymin, ymax, zmin, zmax)
                                            # 47416.755556
## [1] 47416.75556
f3 \leftarrow function(x, y, z)  sqrt(x^2 + y^2)
a <- -2; b <- 2
ymin \leftarrow function(x) - sqrt(4-x^2)
ymax <- function(x)  sqrt(4-x^2)
zmin \leftarrow function(x, y) \quad sqrt(x^2 + y^2)
zmax <- 2
integral3(f3, a, b, ymin, ymax, zmin, zmax)
                                            # 8.377579076269617
## [1] 8.37758
```

164 interp1

# **Description**

One-dimensional interpolation of points.

### Usage

## **Arguments**

Х	Numeric vector; points on the x-axis; at least two points require; will be sorted if necessary.
У	Numeric vector; values of the assumed underlying function; x and y must be of the same length.
xi	Numeric vector; points at which to compute the interpolation; all points must lie between $min(x)$ and $max(x)$ .
method	One of "constant", "linear", "nearest", "spline", or "cubic".

## **Details**

Interpolation to find yi, the values of the underlying function at the points in the vector xi.

Methods can be:

constant	constant between points
linear	linear interpolation (default)
nearest	nearest neighbor interpolation
spline	cubic spline interpolation
cubic	cubic Hermite interpolation

#### Value

Numeric vector representing values at points xi.

## Note

Method 'spline' uses the spline approach by Moler et al., and is identical with the Matlab option of the same name, but slightly different from R's spline function.

The Matlab option "cubic" seems to have no direct correspondence in R. Therefore, we simply use pchip here.

### See Also

```
approx, spline
```

```
x \leftarrow c(0.8, 0.3, 0.1, 0.6, 0.9, 0.5, 0.2, 0.0, 0.7, 1.0, 0.4)
```

interp2

```
y < - x^2
xi <- seq(0, 1, len = 81)
yl <- interp1(x, y, xi, method = "linear")</pre>
yn <- interp1(x, y, xi, method = "nearest")</pre>
ys <- interp1(x, y, xi, method = "spline")</pre>
## Not run:
plot(x, y); grid()
lines(xi, yl, col="blue", lwd = 2)
lines(xi, yn, col="black", lty = 2)
lines(xi, ys, col="red")
## End(Not run)
## Difference between spline (Matlab) and spline (R).
x <- 1:6
y <- c(16, 18, 21, 17, 15, 12)
xs <- linspace(1, 6, 51)
ys <- interp1(x, y, xs, method = "spline")</pre>
sp \leftarrow spline(x, y, n = 51, method = "fmm")
## Not run:
plot(x, y, main = "Matlab and R splines")
grid()
lines(xs, ys, col = "red")
lines(sp$x, sp$y, col = "blue")
legend(4, 20, c("Matlab spline", "R spline"),
              col = c("red", "blue"), lty = 1)
## End(Not run)
```

interp2

Two-dimensional Data Interpolation

## **Description**

Two-dimensional data interpolation similar to a table look-up.

## Usage

```
interp2(x, y, Z, xp, yp, method = c("linear", "nearest", "constant"))
```

# Arguments

х, у	vectors with monotonically increasing elements, representing x- and y-coordinates of the data values in Z.
Z	<pre>numeric length(x)-by-length(y) matrix.</pre>
хр, ур	x-, y-coordinates of points at which interpolated values will be computed.
method	interpolation method, "linear" the most useful.

interp2

### **Details**

Computes a vector containing elements corresponding to the elements of xp and yp, determining by interpolation within the two-dimensional function specified by vectors x and y, and matrix Z.

x and y must be monotonically increasing. They specify the points at which the data Z is given. Therefore, length(x) = nrow(Z) and length(y) = ncol(Z) must be satisfied.

xp and yp must be of the same length.

The functions appears vectorized as xp, yp can be vectors, but internally they are treated in a for loop.

#### Value

Vector the length of xp of interpolated values.

For methods "constant" and "nearest" the intervals are considered closed from left and below. Out of range values are returned as NAs.

#### Note

The corresponding Matlab function has also the methods "cubic" and "spline". If in need of a nonlinear interpolation, take a look at barylag2d in this package and the example therein.

### See Also

```
interp1, barylag2d
```

```
## Not run:
    x <- linspace(-1, 1, 11)
    y <- linspace(-1, 1, 11)
    mgrid <- meshgrid(x, y)
    Z <- mgrid$X^2 + mgrid$Y^2
    xp <- yp <- linspace(-1, 1, 101)

method <- "linear"
    zp <- interp2(x, y, Z, xp, yp, method)
    plot(xp, zp, type = "l", col = "blue")

method = "nearest"
    zp <- interp2(x, y, Z, xp, yp, method)
    lines(xp, zp, col = "red")
    grid()

## End(Not run)</pre>
```

inv 167

inv

Matrix Inverse (Matlab Style)

# Description

Invert a numeric or complex matrix.

# Usage

inv(a)

## **Arguments**

а

real or complex square matrix

## **Details**

Computes the matrix inverse by calling solve(a) and catching the error if the matrix is nearly singular.

### Value

square matrix that is the inverse of a.

## Note

inv() is the function name used in Matlab/Octave.

### See Also

solve

```
A <- hilb(6)
B <- inv(A)
B
# Compute the inverse matrix through Cramer's rule:
n <- nrow(A)
detA <- det(A)
b <- matrix(NA, nrow = n, ncol = n)
for (i in 1:n) {
    for (j in 1:n) {
        b[i, j] <- (-1)^(i+j) * det(A[-j, -i]) / detA
    }
}
b</pre>
```

168 invlap

# **Description**

Numerical inversion of Laplace transforms.

# Usage

```
invlap(Fs, t1, t2, nnt, a = 6, ns = 20, nd = 19)
```

## **Arguments**

Fs	function representing the function to be inverse-transformed.
t1, t2	end points of the interval.
nnt	number of grid points between t1 and t2.
a	shift parameter; it is recommended to preserve value 6.
ns, nd	further parameters, increasing them leads to lower error.

## **Details**

The transform Fs may be any reasonable function of a variable s^a, where a is a real exponent. Thus, the function invlap can solve fractional problems and invert functions Fs containing (ir)rational or transcendental expressions.

### Value

Returns a list with components x the x-coordinates and y the y-coordinates representing the original function in the interval [t1, t2].

### Note

Based on a presentation in the first reference. The function invlap on MatlabCentral (by ) served as guide. The Talbot procedure from the second reference could be an interesting alternative.

### References

- J. Valsa and L. Brancik (1998). Approximate Formulae for Numerical Inversion of Laplace Transforms. Intern. Journal of Numerical Modelling: Electronic Networks, Devices and Fields, Vol. 11, (1998), pp. 153-166.
- L.N.Trefethen, J.A.C.Weideman, and T.Schmelzer (2006). Talbot quadratures and rational approximations. BIT. Numerical Mathematics, 46(3):653–670.

invperm 169

### **Examples**

```
Fs \leftarrow function(s) 1/(s^2 + 1)
                                 # sine function
Li <- invlap(Fs, 0, 2*pi, 100)
## Not run:
plot(Li[[1]], Li[[2]], type = "l", col = "blue"); grid()
Fs <- function(s) tanh(s)/s
                                        # step function
L1 <- invlap(Fs, 0.01, 20, 1000)
plot(L1[[1]], L1[[2]], type = "1", col = "blue")
L2 <- invlap(Fs, 0.01, 20, 2000, 6, 280, 59)
lines(L2[[1]], L2[[2]], col="darkred"); grid()
Fs <- function(s) 1/(sqrt(s)*s)
L1 <- invlap(Fs, 0.01, 5, 200, 6, 40, 20)
plot(L1[[1]], L1[[2]], type = "l", col = "blue"); grid()
Fs \leftarrow function(s) 1/(s^2 - 1)
                                        # hyperbolic sine function
Li <- invlap(Fs, 0, 2*pi, 100)
plot(Li[[1]], Li[[2]], type = "1", col = "blue"); grid()
Fs <- function(s) 1/s/(s + 1)
                                        # exponential approach
Li <- invlap(Fs, 0, 2*pi, 100)
plot(Li[[1]], Li[[2]], type = "l", col = "blue"); grid()
gamma <- 0.577215664901532
                                        # Euler-Mascheroni constant
Fs <- function(s) -1/s * (log(s)+gamma) # natural logarithm
Li <- invlap(Fs, 0, 2*pi, 100)
plot(Li[[1]], Li[[2]], type = "1", col = "blue"); grid()
Fs <- function(s) (20.5+3.7343*s^1.15)/(21.5+3.7343*s^1.15+0.8*s^2.2+0.5*s^0.9)/s
L1 <- invlap(Fs, 0.01, 5, 200, 6, 40, 20)
plot(L1[[1]], L1[[2]], type = "1", col = "blue")
grid()
## End(Not run)
```

invperm

Inverse Permutation

### **Description**

Generates the inverse permutation.

## Usage

invperm(p)

#### **Arguments**

permutation, i.e. the vector 1:n permuted.

170 isempty

## **Details**

Generates the inverse permutation.

#### Value

Vector of permuted elements of 1:length(p).

## See Also

randperm

## **Examples**

```
p1 <- c(1,3,5,2,4)
p1inv <- invperm(p1)  # 1 4 2 5 3

# Define two more functions for permutations
compoperm <- function(p, q) q[p]  # composition of permutations
compoperm(p1, p1inv)  # 1 2 3 4 5
applyperm <- function(p, x) x[p]  # apply permutation to vector
p2 <- c(2,1,3,5,4)
x <- c(11,12,13,14,15)
applyperm(compoperm(p2, p1), x) == applyperm(p2, applyperm(p1, x))  # all TRUE</pre>
```

isempty

isempty Property

## **Description**

Determine if an object is empty.

# Usage

```
isempty(x)
```

## **Arguments**

Х

an R object

#### **Details**

An empty object has length zero.

## Value

TRUE if x has length 0; otherwise, FALSE.

isprime 171

# **Examples**

```
isempty(c(0)) # FALSE isempty(matrix(0, 1, 0)) # TRUE
```

isprime

isprime Property

### **Description**

Vectorized version, returning for a vector or matrix of positive integers a vector of the same size containing 1 for the elements that are prime and 0 otherwise.

## Usage

```
isprime(x)
```

### **Arguments**

Х

vector or matrix of nonnegative integers

#### **Details**

Given an array of positive integers returns an array of the same size of 0 and 1, where the i indicates a prime number in the same position.

### Value

array of elements 0, 1 with 1 indicating prime numbers

# See Also

```
factors, primes
```

```
x <- matrix(1:10, nrow=10, ncol=10, byrow=TRUE)
x * isprime(x)

# Find first prime number octett:
octett <- c(0, 2, 6, 8, 30, 32, 36, 38) - 19
while (TRUE) {
    octett <- octett + 210
    if (all(as.logical(isprime(octett)))) {
        cat(octett, "\n", sep=" ")
        break
    }
}</pre>
```

172 itersolve

|--|--|

## **Description**

Iterative solutions of systems of linear equations.

# Usage

## **Arguments**

A numerical matrix, square and non-singular.

b numerical vector or column vector.

x0 starting solution for iteration; defaults to null vector.

nmax maximum number of iterations.

tol relative tolerance.

method iterative method, Gauss-Seidel, Jacobi, or Richardson.

### **Details**

Iterative methods are based on splitting the matrix A=(P-A)-A with a so-called 'preconditioner' matrix P. The methods differ in how to choose this preconditioner.

#### Value

Returns a list with components x the solution, iter the number of iterations, and method the name of the method applied.

### Note

Richardson's method allows to specify a 'preconditioner'; this has not been implemented yet.

### References

Quarteroni, A., and F. Saleri (2006). Scientific Computing with MATLAB and Octave. Springer-Verlag, Berlin Heidelberg.

### See Also

grSolve

jacobian 173

### **Examples**

```
N <- 10
A <- Diag(rep(3,N)) + Diag(rep(-2, N-1), k=-1) + Diag(rep(-1, N-1), k=1)
b <- A %*% rep(1, N)
x0 <- rep(0, N)

itersolve(A, b, tol = 1e-8, method = "Gauss-Seidel")
# [1] 1 1 1 1 1 1 1 1 1 1
# [1] 87
itersolve(A, b, x0 = 1:10, tol = 1e-8, method = "Jacobi")
# [1] 1 1 1 1 1 1 1 1 1 1 1
# [1] 177</pre>
```

jacobian

Jacobian Matrix

## Description

Jacobian matrix of a function  $R^n -> R^m$ .

## Usage

```
jacobian(f, x0, heps = .Machine$double.eps^(1/3), ...)
```

## **Arguments**

```
f m functions of n variables.

x0 Numeric vector of length n.

heps This is h in the derivative formula.

parameters to be passed to f.
```

## **Details**

Computes the derivative of each funktion  $f_j$  by variable  $x_i$  separately, taking the discrete step h.

### Value

Numeric m-by-n matrix J where the entry J[j, i] is  $\frac{\partial f_j}{\partial x_i}$ , i.e. the derivatives of function  $f_j$  line up in row i for  $x_1, \ldots, x_n$ .

# Note

Obviously, this function is not vectorized.

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

174 kriging

### See Also

gradient

### **Examples**

kriging

Interpolation by Kriging

### **Description**

Simple and ordinary Kriging interpolation and interpolating function.

### Usage

```
kriging(u, v, u0, type = c("ordinary", "simple"))
```

## **Arguments**

u an nxm-matrix of n points in the m-dimensional space.
 v an n-dim. (column) vector of interpolation values.
 u0 a kxm-matrix of k points in R^m to be interpolated.
 type character; values 'simple' or 'ordinary'; no partial matching.

#### **Details**

Kriging is a geo-spatial estimation procedure that estimates points based on the variations of known points in a non-regular grid. It is especially suited for surfaces.

### Value

kriging returns a k-dim. vektor of interpolation values.

## Note

In the literature, different versions and extensions are discussed.

### References

Press, W. H., A. A. Teukolsky, W. T. Vetterling, and B. P. Flannery (2007). Numerical recipes: The Art of Scientific Computing (3rd Ed.). Cambridge University Press, New York, Sect. 3.7.4, pp. 144-147. http://apps.nrbook.com/empanel/index.html?pg=144#

kron 175

### See Also

akimaInterp, barylag2d, package kriging

```
## Interpolate the Saddle Point function
f \leftarrow function(x) x[1]^2 - x[2]^2
                                    # saddle point function
set.seed(8237)
n <- 36
x \leftarrow c(1, 1, -1, -1, runif(n-4, -1, 1)) \# add four vertices
y \leftarrow c(1, -1, 1, -1, runif(n-4, -1, 1))
u \leftarrow cbind(x, y)
v <- numeric(n)</pre>
for (i in 1:n) v[i] \leftarrow f(c(x[i], y[i]))
                                              #=> 0.006177183
kriging(u, v, c(0, 0))
                                              #=> 0.006229557
kriging(u, v, c(0, 0), type = "simple")
## Not run:
xs <- linspace(-1, 1, 101)
                                          # interpolation on a diagonal
u0 <- cbind(xs, xs)</pre>
yo <- kriging(u, v, u0, type = "ordinary") # ordinary kriging
ys <- kriging(u, v, u0, type = "simple") # simple kriging
plot(xs, ys, type = "l", col = "blue", ylim = c(-0.1, 0.1),
             main = "Kriging interpolation along the diagonal")
lines(xs, yo, col = "red")
legend( -1.0, 0.10, c("simple kriging", "ordinary kriging", "function"),
        lty = c(1, 1, 1), lwd = c(1, 1, 2), col=c("blue", "red", "black"))
grid()
lines(c(-1, 1), c(0, 0), lwd = 2)
## End(Not run)
## Find minimum of the sphere function
f \leftarrow function(x, y) x^2 + y^2 + 100
v \leftarrow bsxfun(f, x, y)
ff <- function(w) kriging(u, v, w)</pre>
ff(c(0, 0))
                                              #=> 100.0317
## Not run:
optim(c(0.0, 0.0), ff)
# $par: [1] 0.04490075 0.01970690
# $value: [1] 100.0291
ezcontour(ff, c(-1, 1), c(-1, 1))
points(0.04490075, 0.01970690, col = "red")
## End(Not run)
```

176 L1linreg

# **Description**

Kronecker tensor product of two matrices.

## Usage

```
kron(a, b)
```

## **Arguments**

a real or complex matrixb real or complex matrix

### **Details**

The Kronecker product is a large matrix formed by all products between the elements of a and those of b. The first left block is a11\*b, etc.

### Value

```
an (n*p \times m*q-matrix, if a is (n \times m and b is (p \times q)).
```

## Note

kron() is an alias for the R function kronecker(), which can also be executed with the binary operator '%x%'.

## **Examples**

```
a <- diag(1, 2, 2)
b <- matrix(1:4, 2, 2)
kron(a, b)
kron(b, a)</pre>
```

L1linreg

L1 Linear Regression

## **Description**

Solve the linear system  $A \times b$  in an Lp sense, that is minimize the term sum  $|b - A \times p|$ . The case p=1 is also called "least absolute deviation" (LAD) regression.

# Usage

```
L1linreg(A, b, p = 1, tol = 1e-07, maxiter = 200)
```

L1linreg 177

#### **Arguments**

A	matrix of independent variables.
b	independent variables.
p	the p in $L^p$ norm, p<=1.
tol	relative tolerance.
maxiter	maximum number of iterations.

### **Details**

L1/Lp regression is here solved applying the "iteratively reweighted least square" (IRLS) method in which each step involves a weighted least squares problem.

If an intercept term is required, add a unit column to A.

### Value

Returns a list with components x the linear coefficients describing the solution, reltol the relative tolerance reached, and niter the number of iterations.

### Note

In this case of p=1, the problem would be better approached by use of linear programming methods.

### References

Dasgupta, M., and S.K. Mishra (2004). Least absolute deviation estimation of linear econometric models: A literature review. MPRA Paper No. 1781.

URL:http://mpra.ub.uni-muenchen.de/1781/1/MPRA\_paper\_1781.pdf

## See Also

```
lm, lsqnonlin, quantreg::rq
```

```
m <- 101; n <- 10  # no. of data points, degree of polynomial
x <- seq(-1, 1, len=m)
y <- runge(x)  # Runge's function
A <- outer(x, n:0, '^') # Vandermonde matrix
b <- y

( sol <- L1linreg(A, b) )
# $x
# [1] -21.93242  0.00000 62.91092  0.00000 -67.84854  0.00000
# [7] 34.14400  0.00000 -8.11899  0.00000  0.84533
#
# $reltol
# [1] 6.712355e-10
#
# $niter</pre>
```

178 laguerre

```
# [1] 81
# minimum value of polynomial L1 regression
sum(abs(polyval(sol$x, x) - y))
# [1] 3.061811
```

laguerre

Laguerre's Method

### **Description**

Laguerre's method for finding roots of complex polynomials.

## Usage

```
laguerre(p, x0, nmax = 25, tol = .Machine$double.eps^(1/2))
```

## **Arguments**

p real or complex vector representing a polynomial.

x0 real or complex point near the root.

nmax maximum number of iterations.

tol absolute tolerance.

#### **Details**

Uses values of the polynomial and its first and second derivative.

### Value

The root found, or a warning about the number of iterations.

## Note

Computations are caried out in complex arithmetic, and it is possible to obtain a complex root even if the starting estimate is real.

### References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

#### See Also

roots

lambertWp 179

## **Examples**

```
# 1 x^5 - 5.4 x^4 + 14.45 x^3 - 32.292 x^2 + 47.25 x - 26.46 p <- c(1.0, -5.4, 14.45, -32.292, 47.25, -26.46) laguerre(p, 1) #=> 1.2 laguerre(p, 2) #=> 2.099987 (should be 2.1) laguerre(p, 2i) #=> 0+2.236068i (+- 2.2361i, i.e sqrt(-5))
```

lambertWp

Lambert's W Function

## **Description**

Principal real branch of the Lambert W function.

## Usage

```
lambertWp(x)
lambertWn(x)
```

### **Arguments**

Х

Numeric vector of real numbers  $\geq -1/e$ .

#### **Details**

The Lambert W function is the inverse of  $x \rightarrow x e^x$ , with two real branches, W0 for  $x \ge -1/e$  and W-1 for  $-1/e \le x \le 0$ . Here the principal branch is called lambertWp, the other one lambertWp, computed for real x.

The value is calculated using an iteration that stems from applying Halley's method. This iteration is quite fast and accurate.

The functions is not really vectorized, but at least returns a vector of values when presented with a numeric vector of length >= 2.

## Value

Returns the solution w of w\*exp(w) = x for real x with NaN if x < 1/exp(1) (resp. x >= 0 for the second branch).

#### Note

See the examples how values for the second branch or the complex Lambert W function could be calculated by Newton's method.

### References

Corless, R. M., G. H.Gonnet, D. E. G Hare, D. J. Jeffrey, and D. E. Knuth (1996). On the Lambert W Function. Advances in Computational Mathematics, Vol. 5, pp. 329-359. http://www.apmaths.uwo.ca/~djeffrey/0ffprints/W-adv-cm.pdf.

180 laplacian

## See Also

hallev

```
## Examples
lambertWp(0)
                     #=> 0
lambertWp(1)
                     #=> 0.5671432904097838... Omega constant
lambertWp(exp(1))
                      #=> 1
lambertWp(-log(2)/2) #=> -log(2)
# The solution of x * a^x = z is W(\log(a)*z)/\log(a)
\# x * 123^{(x-1)} = 3
lambertWp(3*123*log(123))/log(123) #=> 1.19183018...
x <- seq(-0.35, 0.0, by=0.05)
w <- lambertWn(x)</pre>
w * exp(w)
                    # max. error < 3e-16
# [1] -0.35 -0.30 -0.25 -0.20 -0.15 -0.10 -0.05 NaN
## Not run:
xs <- c(-1/exp(1), seq(-0.35, 6, by=0.05))
ys <- lambertWp(xs)</pre>
plot(xs, ys, type="1", col="darkred", lwd=2, ylim=c(-2,2),
     main="Lambert W0 Function", xlab="", ylab="")
grid()
points(c(-1/exp(1), 0, 1, exp(1)), c(-1, 0, lambertWp(1), 1))
text(1.8, 0.5, "Omega constant")
## End(Not run)
## Analytic derivative of lambertWp (similar for lambertWn)
D_lambertWp <- function(x) {</pre>
   xw <- lambertWp(x)</pre>
    1 / (1+xw) / exp(xw)
D_{\text{lambertWp}}(c(-1/\exp(1), 0, 1, \exp(1)))
# [1] Inf 1.0000000 0.3618963 0.1839397
## Second branch resp. the complex function lambertWm()
F <- function(xy, z0) {
   z \leftarrow xy[1] + xy[2]*1i
   fz <- z * exp(z) - z0
    return(c(Re(fz), Im(fz)))
}
newtonsys(F, c(-1, -1), z0 = -0.1) #=> -3.5771520639573
newtonsys(F, c(-1, -1), z0 = -pi/2) #=> -1.5707963267949i = -pi/2 * 1i
```

laplacian 181

# Description

Numerically compute the Laplacian of a function.

### Usage

```
laplacian(f, x0, h = .Machine$double.eps^(1/4), ...)
```

### **Arguments**

```
f univariate function of several variables.
```

x0 point in  $\mathbb{R}^n$ .

h step size.

... variables to be passed to f.

### **Details**

Computes the Laplacian operator  $f_{x_1x_1} + \ldots + f_{x_nx_n}$  based on the three-point central difference formula, expanded to this special case.

Assumes that the function has continuous partial derivatives.

# Value

Real number.

# References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

### See Also

hessian

```
f <- function(x) x[1]^2 + 2*x[1]*x[2] + x[2]^2 laplacian(f, c(1,1))
```

182 lebesgue

Lebesgue Constant

# Description

Estimates the Lebesgue constant.

#### Usage

```
lebesgue(x, refine = 4, plotting = FALSE)
```

### **Arguments**

x numeric vector of grid points

refine refine the grid with 2^refine grid points; can only be an integer between 2 and

10, default 4.

plotting shall the Lebesgue function be plotted.

#### **Details**

The Lebesgue constant gives an estimation  $||P_n f|| \le L||f||$  (in minimax norm) where  $P_n f$  is the interpolating polynomial of order n for f on an interval [a, b].

### Value

Lebesgue constant for the given grid points.

#### Note

The Lebesgue constant plays an important role when estimating the distance of interpolating polynomials from the minimax solution (see the Remez algorithm).

### References

Berrut, J.-P., and L. Nick Trefethen (2004). "Barycentric Lagrange Interpolation". SIAM Review, Vol. 46(3), pp.501–517.

### See Also

barylag

```
lebesgue(seq(0, 1, length.out = 6)) #=> 3.100425
```

legendre 183

legendre

Legendre Functions (Matlab Style)

### **Description**

Calculate the values of (associated) Legendre functions.

#### Usage

```
legendre(n, x)
```

#### **Arguments**

- n degree of the Legendre polynomial involved.
- x real points to evaluate Legendre's functions at.

#### **Details**

legendre (n,x) computes the associated Legendre functions of degree n and order  $m=0,1,\ldots,n$ , evaluated for each element of x where x must contain real values in [-1,1].

If x is a vector, then L=legendre(n,x) is an (n+1)-by-N matrix, where N=length(x). Each element L[m+1,i] corresponds to the associated Legendre function of degree legendre(n,x) and order m evaluated at x[i].

Note that the first row of L is the Legendre polynomial evaluated at x.

### Value

Returns a matrix of size (n+1)-by-N where N=length(x).

#### Note

Legendre functions are solutions to Legendre's differential equation (it occurs when solving Laplace's equation in spherical coordinates).

### See Also

```
chebPoly
```

```
x <- c(0.0, 0.1, 0.2)
legendre(2, x)
# [,1] [,2] [,3]
# [1,] -0.5 -0.4850000 -0.4400000
# [2,] 0.0 -0.2984962 -0.5878775
# [3,] 3.0 2.9700000 2.8800000
## Not run:</pre>
```

line\_integral

line\_integral

*Line integral (in the complex plane)* 

## Description

Provides complex line integrals.

### Usage

```
line_integral(fun, waypoints, method = NULL, reltol = 1e-8, ...)
```

### **Arguments**

fun integrand, complex (vectorized) function.

method integration procedure, see below.

waypoints complex integration: points on the integration curve.

reltol relative tolerance.

... additional parameters to be passed to the function.

### **Details**

line\_integral realizes complex line integration, in this case straight lines between the waypoints. By passing discrete points densely along the curve, arbitrary line integrals can be approximated.

line\_integral will accept the same methods as integral; default is integrate from Base R.

#### Value

Returns the integral, no error terms given.

#### See Also

integral

linprog 185

#### **Examples**

```
## Complex integration examples
points <- c(0, 1+1i, 1-1i, 0)
                                           # direction mathematically negative
f \leftarrow function(z) 1 / (2*z -1)
I <- line_integral(f, points)</pre>
                                           # 0 ; residuum 2 pi 1i * 1/2
abs(I - (0-pi*1i))
f \leftarrow function(z) 1/z
points <- c(-1i, 1, 1i, -1, -1i)
I <- line_integral(f, points)</pre>
                                           # along a rectangle around 0+0i
abs(I - 2*pi*1i)
                                           #=> 0 ; residuum: 2 pi i * 1
N <- 100
x \leftarrow linspace(0, 2*pi, N)
y < -\cos(x) + \sin(x)*1i
J <- line_integral(f, waypoints = y)</pre>
                                           # along a circle around 0+0i
abs(I - J)
                                           #=> 5.015201e-17; same residuum
```

linprog

Linear Programming Solver

#### **Description**

Solves simple linear programming problems, allowing for inequality and equality constraints as well as lower and upper bounds.

### Usage

```
linprog(cc, A = NULL, b = NULL, Aeq = NULL, beq = NULL,
    lb = NULL, ub = NULL, x0 = NULL, I0 = NULL,
    bigM = 100, maxiter = 20, maximize = FALSE)
```

#### **Arguments**

СС	defines the linear objective function.
A	matrix representing the inequality constraints A $x \le b$ .
b	vector, right hand side of the inequalities.
Aeq	matrix representing the equality constraints Aeq $x \le beq$ .
beq	vector, right hand side of the inequalities.
lb	lower bounds, if not NULL must all be greater or equal 0.
ub	upper bounds, if not NULL must all be greater or equal 1b.
x0	feasible base vector, will not be used at the moment.
10	index set of x0, will not be used at the moment.
bigM	big-M constant, will be used for finding a base vector.
maxiter	maximum number of iterations.
maximize	logical; shall the objective be minimized or maximized?

186 linprog

#### **Details**

Solves linear programming problems of the form mincc' \* x such that

$$A * x \le b$$
$$A_{eq} * x = b_{eq}$$
$$lb \le x \le ub$$

#### Value

List with

- x the solution vector.
- fval the value at the optimal solution.
- errno, mesage the error number and message.

#### Note

This is a first version that will be unstable at times. For real linear programming problems use package lpSolve.

#### Author(s)

HwB < hwborchers@googlemail.com>

#### References

Vanderbei, R. J. (2001). Linear Programming: Foundations and Extensions. Princeton University Press.

Eiselt, H. A., and C.-L. Sandblom (2012). Operations Research: A Model-based Approach. Springer-Verlag, Berlin Heidelberg.

#### See Also

```
linprog::solveLP, lpSolve::lp
```

linprog 187

```
Ain \leftarrow matrix(c(-250, -380, -257,
                                           250, 380, 257,
                                            13, 31, 28), 3, 3, byrow = TRUE)
bin <- c(-1800, 2200, 100)
linprog(cc, A = Ain, b = bin)
#-- employee scheduling
cc \leftarrow c(1, 1, 1, 1, 1, 1)
A \leftarrow (-1)*matrix(c(1, 0, 0, 0, 0, 1,
                                               1, 1, 0, 0, 0, 0,
                                                0, 1, 1, 0, 0, 0,
                                               0, 0, 1, 1, 0, 0,
                                                0, 0, 0, 1, 1, 0,
                                                0, 0, 0, 0, 1, 1), 6, 6, byrow = TRUE)
b <- -c(17, 9, 19, 12, 5, 8)
linprog(cc, A, b)
#-- inventory models
cc <- c(1, 1.1, 1.2, 1.25, 0.05, 0.15, 0.15)
Aeq <- matrix(c(1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, 0, -1, 0, -1, 0, 0, -1, 0, -1, 0, -1, 0, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, -1, 0, 
                                        0, 1, 0, 0, 1, -1, 0,
                                        0, 0, 1, 0, 0, 1, -1,
                                        0, 0, 0, 1, 0, 0, 1), 4, 7, byrow = TRUE)
beq <- c(60, 70, 130, 150)
ub <- c(120, 140, 150, 140, Inf, Inf, Inf)
linprog(cc, Aeq = Aeq, beq = beq, ub = ub)
#-- allocation problem
cc <- c(1, 1, 1, 1, 1)
A \leftarrow matrix(c(-5,
                                              0,
                                                                    0,
                                                                                   0,
                                                                                                  0,
                                     0, -4.5,
                                                              0,
                                                                                  0,
                                                                                                  0,
                                      0,
                                                 0, -5.5,
                                                                                  0,
                                                                                                  0,
                                                    0,
                                                                    0, -3.5,
                                                                                                  0,
                                                     0,
                                                                    0,
                                                                                   0, -5.5,
                                                                                  0,
                                                    0,
                                                                    0,
                                                                                                  0,
                                      0,
                                              4.5,
                                                              0,
                                                                                   0,
                                                                                                  0,
                                                   0, 5.5,
                                      0,
                                                                                  0,
                                                                                                  0,
                                                               0, 3.5,
                                     0,
                                                    0,
                                                                                                  0,
                                                                                   0, 5.5,
                                                   0,
                                                                    0,
                                   -5, -4.5, -5.5, -3.5, -5.5,
                                   10, 10.0, 10.0, 10.0, 10.0,
                                   0.2, 0.2, 0.2, -1.0, 0.2), 13, 5, byrow = TRUE)
b <- c(-50, -55, -60, -50, -50, rep(100, 5), -5*64, 700, 0)
# linprog(cc, A = A, b = b)
lb <- b[1:5] / diag(A[1:5, ])</pre>
ub \leftarrow b[6:10] / diag(A[6:10, ])
A1 \leftarrow A[11:13,]
b1 <- b[11:13]
linprog(cc, A1, b1, lb = lb, ub = ub)
#-- transportation problem
cc \leftarrow c(1, 7, 4, 2, 3, 5)
```

linspace

```
0, 0, 0, 1, 1, 1,

1, 0, 0, 1, 0, 0,

0, 1, 0, 0, 1, 0,

0, 0, 1, 0, 0, 1), 5, 6, byrow = TRUE)

beq <- c(30, 20, 15, 25, 10)

linprog(cc, Aeq = Aeq, beq = beq)
```

linspace

Linearly Spaced Sequences

# Description

Generate linearly spaced sequences.

# Usage

```
linspace(x1, x2, n = 100)
```

# Arguments

x1	numeric scalar specifying starting point
x2	numeric scalar specifying ending point
n	numeric scalar specifying number of points to be generated

#### **Details**

These functions will generate n linearly spaced points between x1 and x2.

If n < 2, the result will be the ending point x2.

## Value

vector containing n points between x1 and x2 inclusive.

### See Also

```
logspace, seq
```

```
linspace(1, 10, 9)
```

logspace 189

logspace

Log-linearly Spaced Sequences

# Description

Generate log-linearly spaced sequences.

# Usage

```
logspace(x1, x2, n = 50)
logseq(x1, x2, n = 100)
```

# Arguments

x1	numeric scalar specifying starting point
x2	numeric scalar specifying ending point
n	numeric scalar specifying number of points to be generated

#### **Details**

These functions will generate logarithmically resp. exponentially spaced points between x1 and x2 resp.  $10^x1$  and  $10^x2$ .

If n < 2, the result will be the ending point x2. For logspace(), if x2 = pi, the endpoint will be pi and not 10^pi!

### Value

vector containing n points between x1 and x2 inclusive.

# See Also

```
logspace, seq
```

```
logspace(1, pi, 36)
logseq(0.05, 1, 20)
```

190 lsqlin

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Linear Least-Squares Fitting

### **Description**

Solves linearly constrained linear least-squares problems.

### Usage

```
lsqlin(A, b, C, d, tol = 1e-13)
```

## Arguments

Α	nxm-matrix defining the least-squares problem.
b	vector or colum matrix with n rows; when it has more than one column it describes several least-squares problems.
С	pxm-matrix for the constraint system.
d	vector or px1-matrix, right hand side for the constraints.
tol	tolerance to be passed to pinv.

#### **Details**

lsqlin(A, b, C, d) minimizes ||A\*x - b|| (i.e., in the least-squares sense) subject to C\*x = d.

#### Value

Returns a least-squares solution as column vector, or a matrix of solutions in the columns if b is a matrix with several columns.

### Note

The Matlab function lsqlin solves a more general problem, allowing additional linear inequalities and bound constraints. In R, bound constraints could be treated using function transfinite in package 'adagio'. Linear inequalities will be added later applying Linear Algebra methods alone.

### Author(s)

HwB email: <a href="mailto:</a> email: <a href="mailto:</a> googlemail.com>

### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Society for Industrial and Applied Mathematics, Philadelphia.

#### See Also

nullspace, pinv

lsqlin 191

```
A <- matrix(c(
               0.1576,
    0.8147,
                           0.6557,
               0.9706,
    0.9058,
                           0.0357,
    0.1270,
               0.9572,
                           0.8491,
               0.4854,
    0.9134,
                           0.9340,
    0.6324,
               0.8003,
                           0.6787,
    0.0975,
               0.1419,
                           0.7577,
               0.4218,
                           0.7431,
    0.2785,
    0.5469,
               0.9157,
                           0.3922,
    0.9575,
               0.7922,
                           0.6555,
    0.9649,
               0.9595,
                           0.1712), 10, 3, byrow = TRUE)
b <- matrix(c(</pre>
    0.7060,
               0.4387,
    0.0318,
               0.3816,
    0.2769,
               0.7655,
               0.7952,
    0.0462,
    0.0971,
               0.1869,
    0.8235,
               0.4898,
    0.6948,
               0.4456,
    0.3171,
               0.6463,
    0.9502,
               0.7094,
    0.0344,
               0.7547), 10, 2, byrow = TRUE)
C <- matrix(c(
    1.0000,
               1.0000,
                           1.0000,
    1.0000,
              -1.0000,
                           0.5000), 2, 3, byrow = TRUE)
d <- as.matrix(c(1, 0.5))
# With a full rank constraint system
(L \leftarrow lsqlin(A, b, C, d))
# 0.10326838 0.3740381
# 0.03442279 0.1246794
# 0.86230882 0.5012825
C %*% L
# 1.0 1.0
# 0.5 0.5
## Not run:
# With a rank deficient constraint system
C <- str2num('[1 1 1;1 1 1]')</pre>
d <- str2num('[1;1]')</pre>
(L <- lsqlin(A, b[, 1], C, d))
# 0.2583340
# -0.1464215
# 0.8880875
C %*% L
                # 1 1 as column vector
# Where both A and C are rank deficient
A2 \leftarrow repmat(A[, 1:2], 1, 2)
C \leftarrow ones(2, 4) \# d as above
(L <- lsqlin(A2, b[, 2], C, d))
# 0.2244121
```

192 Isqnonlin

lsqnonlin

Nonlinear Least-Squares Fitting

## Description

1sqnonlin solves nonlinear least-squares problems, including nonlinear data-fitting problems, through the Levenberg-Marquardt approach.

1sqnonneg solve nonnegative least-squares constraints problem.

#### Usage

```
lsqnonlin(fun, x0, options = list(), ...)
lsqnonneg(C, d)

lsqsep(flist, p0, xdata, ydata, const = TRUE)
lsqcurvefit(fun, p0, xdata, ydata)
```

### **Arguments**

fun	User-defined, vector-valued function.
x0	starting point.
	additional parameters passed to the function.
options	list of options, for details see below.
C, d	matrix and vector such that $C \times - d$ will be minimized with $x \ge 0$ .
flist	list of (nonlinear) functions, depending on one extra parameter.
p0	starting parameters.
xdata, ydata	data points to be fitted.
const	logical; shall a constant term be included.

#### **Details**

Isononlin computes the sum-of-squares of the vector-valued function fun, that is if  $f(x) = (f_1(x), \dots, f_n(x))$  then

$$min||f(x)||_2^2 = min(f_1(x)^2 + \ldots + f_n(x)^2)$$

will be minimized.

x=1 sqnonlin(fun, x0) starts at point x0 and finds a minimum of the sum of squares of the functions described in fun. fun shall return a vector of values and not the sum of squares of the values. (The algorithm implicitly sums and squares fun(x).)

options is a list with the following components and defaults:

Isqnonlin 193

- tau: used as starting value for Marquardt parameter.
- tolx: stopping parameter for step length.
- tolg: stopping parameter for gradient.
- maxeval the maximum number of function evaluations.

Typical values for tau are from 1e-6...1e-3...1 with small values for good starting points and larger values for not so good or known bad starting points.

1sqnonneg solves the linear least-squares problem  $C \times - d$ , x nonnegative, treating it through an active-set approach..

1sqsep solves the separable least-squares fitting problem

```
y = a0 + a1*f1(b1, x) + ... + an*fn(bn, x)
```

where fi are nonlinear functions each depending on a single extra paramater bi, and ai are additional linear parameters that can be separated out to solve a nonlinear problem in the bi alone.

lsqcurvefit is simply an application of lsqnonlin to fitting data points. fun(p, x) must be a function of two groups of variables such that p will be varied to minimize the least squares sum, see the example below.

#### Value

1sqnonlin returns a list with the following elements:

- x: the point with least sum of squares value.
- ssq: the sum of squares.
- ng: norm of last gradient.
- nh: norm of last step used.
- mu: damping parameter of Levenberg-Marquardt.
- neval: number of function evaluations.
- errno: error number, corresponds to error message.
- errmess: error message, i.e. reason for stopping.

1sqnonneg returns a list of x the non-negative solition, and resid.norm the norm of the residual.

lsqsep will return the coefficients sparately, a0 for the constant term (being 0 if const=FALSE) and the vectors a and b for the linear and nonlinear terms, respectively.

### Note

The refined approach, Fletcher's version of the Levenberg-Marquardt algorithm, may be added at a later time; see the references.

#### References

Madsen, K., and H. B.Nielsen (2010). Introduction to Optimization and Data Fitting. Technical University of Denmark, Intitute of Computer Science and Mathematical Modelling.

Lawson, C.L., and R.J. Hanson (1974). Solving Least-Squares Problems. Prentice-Hall, Chapter 23, p. 161.

Fletcher, R., (1971). A Modified Marquardt Subroutine for Nonlinear Least Squares. Report AERE-R 6799, Harwell.

194 Isqnonlin

#### See Also

nlm, nls

```
## Rosenberg function as least-squares problem
x0 < -c(0, 0)
fun <- function(x) c(10*(x[2]-x[1]^2), 1-x[1])
lsqnonlin(fun, x0)
## Example from R-help
y \leftarrow c(5.5199668, 1.5234525, 3.3557000, 6.7211704, 7.4237955, 1.9703127,
       4.3939336, -1.4380091, 3.2650180, 3.5760906, 0.2947972, 1.0569417)
x \leftarrow c(1, 0, 0, 4, 3, 5, 12, 10, 12, 100, 100, 100)
# Define target function as difference
f <- function(b)</pre>
     b[1] * (exp((b[2] - x)/b[3]) * (1/b[3]))/(1 + exp((b[2] - x)/b[3]))^2 - y
x0 <- c(21.16322, 8.83669, 2.957765)
                      # ssq 50.50144 at c(36.133144, 2.572373, 1.079811)
lsqnonlin(f, x0)
# nls() will break down
# nls(Y \sim a*(exp((b-X)/c)*(1/c))/(1 + exp((b-X)/c))^2,
      start=list(a=21.16322, b=8.83669, c=2.957765), algorithm = "plinear")
# Error: step factor 0.000488281 reduced below 'minFactor' of 0.000976563
## Example: Hougon function
x1 <- c(470, 285, 470, 470, 470, 100, 100, 470, 100, 100, 100, 285, 285)
x2 <- c(300, 80, 300, 80, 80, 190, 80, 190, 300, 300, 80, 300, 190)
x3 <- c( 10, 10, 120, 120, 10, 10, 65, 65, 54, 120, 120, 10, 120)
rate < c(8.55, 3.79, 4.82, 0.02, 2.75, 14.39, 2.54,
          4.35, 13.00, 8.50, 0.05, 11.32, 3.13)
fun <- function(b)</pre>
        (b[1]*x2 - x3/b[5])/(1 + b[2]*x1 + b[3]*x2 + b[4]*x3) - rate
lsqnonlin(fun, rep(1, 5))
       [1.25258502 0.06277577 0.04004772 0.11241472 1.19137819]
# $ssq 0.298901
## Example for lsqnonneg()
C1 <- matrix( c(0.1210, 0.2319, 0.4398, 0.9342, 0.1370,
                0.4508, 0.2393, 0.3400, 0.2644, 0.8188,
                0.7159, 0.0498, 0.3142, 0.1603, 0.4302,
                0.8928, 0.0784, 0.3651, 0.8729, 0.8903,
                0.2731, 0.6408, 0.3932, 0.2379, 0.7349,
                0.2548, 0.1909, 0.5915, 0.6458, 0.6873,
                0.8656, 0.8439, 0.1197, 0.9669, 0.3461,
                0.2324, 0.1739, 0.0381, 0.6649, 0.1660,
                0.8049, 0.1708, 0.4586, 0.8704, 0.1556,
                0.9084, 0.9943, 0.8699, 0.0099, 0.1911), ncol = 5, byrow = TRUE)
C2 <- C1 - 0.5
d < -c(0.4225, 0.8560, 0.4902, 0.8159, 0.4608,
       0.4574, 0.4507, 0.4122, 0.9016, 0.0056)
( sol <- lsqnonneg(C1, d) ) #-> resid.norm 0.3694372
```

Iu 195

```
( sol <- lsqnonneg(C2, d) )</pre>
                                #-> $resid.norm 2.863979
## Example for lsqcurvefit()
   Lanczos1 data (artificial data)
f(x) = 0.0951 \times exp(-x) + 0.8607 \times exp(-3 \times x) + 1.5576 \times exp(-5 \times x)
x <- linspace(0, 1.15, 24)
y < -c(2.51340000, 2.04433337, 1.66840444, 1.36641802, 1.12323249, 0.92688972,
       0.76793386, 0.63887755, 0.53378353, 0.44793636, 0.37758479, 0.31973932,
       0.27201308, 0.23249655, 0.19965895, 0.17227041, 0.14934057, 0.13007002,
       0.11381193, 0.10004156, 0.08833209, 0.07833544, 0.06976694, 0.06239313)
p0 <- c(1.2, 0.3, 5.6, 5.5, 6.5, 7.6)
fp \leftarrow function(p, x) p[1]*exp(-p[2]*x) + p[3]*exp(-p[4]*x) + p[5]*exp(-p[6]*x)
lsqcurvefit(fp, p0, x, y)
## Example for lsqsep()
f \leftarrow function(x) 0.5 + x^-0.5 + exp(-0.5*x)
set.seed(8237); n <- 15
x \leftarrow sort(0.5 + 9*runif(n))
                                   y < f(x) + 0.01 \times rnorm(n)
y \leftarrow f(x)
m <- 2
f1 \leftarrow function(b, x) x^b
f2 \leftarrow function(b, x) \exp(b*x)
flist <- list(f1, f2)
start <- c(-0.25, -0.75)
sol \leftarrow lsqsep(flist, start, x, y, const = TRUE)
a0 <- sol$a0; a <- sol$a; b <- sol$b
fsol \leftarrow function(x) \ a0 + a[1]*f1(b[1], x) + a[2]*f2(b[2], x)
## Not run:
    ezplot(f, 0.5, 9.5, col = "gray")
    points(x, y, col = "blue")
    xs <- linspace(0.5, 9.5, 51)
    ys <- fsol(xs)
    lines(xs, ys, col = "red")
## End(Not run)
```

LU Matrix Factorization

# Description

lu

LU decomposition of a positive definite matrix as Gaussian factorization.

### Usage

```
lu(A, scheme = c("kji", "jki", "ijk"))
```

196 lu

```
lufact(A)
lusys(A, b)
```

#### **Arguments**

A square positive definite numeric matrix (will not be checked).

scheme order of row and column operations.

b right hand side of a linear system of equations.

#### **Details**

For a given matrix A, the LU decomposition exists and is unique iff its principal submatrices of order i=1,...,n-1 are nonsingular. The procedure here is a simple Gauss elimination with or without pivoting.

The scheme abbreviations refer to the order in which the cycles of row- and column-oriented operations are processed. The "ijk" scheme is one of the two compact forms, here the Doolite factorization (the Crout factorization would be similar).

lufact applies partial pivoting (along the rows). lusys uses LU factorization to solve the linear system A\*x=b.

#### Value

lu returns a list with components L and U, the two lower and upper triangular matrices such that A=L%\*%U.

lufact returns a list with L and U combined into one matrix LU, the rows used in partial pivoting, and det representing the determinant of A. See the examples how to extract matrices L and U from LU.

lusys returns the solution of the system as a column vector.

#### Note

This function is not meant to process huge matrices or linear systems of equations. Without pivoting it may also be harmed by considerable inaccuracies.

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second edition, Springer-Verlag, Berlin Heidelberg.

J.H. Mathews and K.D. Fink (2003). Numerical Methods Using MATLAB. Fourth Edition, Pearson (Prentice-Hall), updated 2006.

#### See Also

qr

magic 197

#### **Examples**

```
A <- magic(5)
D \leftarrow lu(A, scheme = "ijk")
                         # Doolittle scheme
D$L %*% D$U
       [,1] [,2] [,3] [,4] [,5]
## [1,] 17 24 1 8 15
## [2,] 23 5 7 14 16
        4 6 13 20 22
## [3,]
## [4,] 10 12 19 21
                          3
## [5,] 11 18 25
                         9
H4 <- hilb(4)
lufact(H4)$det
## [1] 0.0000001653439
x0 < -c(1.0, 4/3, 5/3, 2.0)
b <- H4 %*% x0
lusys(H4, b)
          [,1]
## [1,] 1.000000
## [2,] 1.333333
## [3,] 1.666667
## [4,] 2.000000
```

magic

Magic Square

# Description

Create a magic square.

# Usage

magic(n)

#### **Arguments**

n

numeric scalar specifying dimensions for the result; n must be a scalar greater than or equal to 3.

### **Details**

A magic square is a square matrix where all row and column sums and also the diagonal sums all have the same value.

This value or the characteristic sum for a magic square of order n is  $sum(1:n^2)/n$ .

#### Value

Returns an n-by-n matrix constructed from the integers 1 through N^2 with equal row and column sums.

198 meshgrid

### Note

A magic square, scaled by its magic sum, is doubly stochastic.

#### Author(s)

P. Roebuck <roebuck@mdanderson.org> for the first R version in the package 'matlab'. The version here is more R-like.

# **Examples**

```
magic(3)
```

matlab

Matlab Compatibility

# Description

Matlab compatibility.

#### Usage

```
matlab()
```

### **Details**

Lists all the functions and function names that emulate Matlab functions.

#### Value

Invisible NULL value.

meshgrid

Generate a Mesh Grid

# Description

Generate two matrices for use in three-dimensional plots.

# Usage

```
meshgrid(x, y = x)
```

#### **Arguments**

x numerical vector, represents points along the x-axis.

y numerical vector, represents points along the y-axis.

mexpfit 199

### **Details**

The rows of the output array X are copies of the vector x; columns of the output array Y are copies of the vector y.

### Value

Returns two matrices as a list with X and Y components.

#### Note

The three-dimensional variant meshgrid(x, y, z) is not yet implemented.

### See Also

outer

### **Examples**

```
meshgrid(1:5)$X
meshgrid(c(1, 2, 3), c(11, 12))
```

mexpfit

Multi-exponential Fitting

# Description

Multi-exponential fitting means fitting of data points by a sum of (decaying) exponential functions, with or without a constant term.

# Usage

```
mexpfit(x, y, p0, w = NULL, const = TRUE, options = list())
```

### **Arguments**

x, y	x-, y-coordinates of data points to be fitted.
p0	starting values for the exponentials alone; can be positive or negative, but not zero.
W	weight vector; not used in this version.
const	logical; shall an absolute term be included.
options	list of options for lsqnonlin, see there.

200 mexpfit

#### **Details**

The multi-exponential fitting problem is solved here with with a separable nonlinear least-squares approach. If the following function is to be fitted,

$$y = a_0 + a_1 e^{b_1 x} + \ldots + a_n e^{b_n x}$$

it will be looked at as a nonlinear optimization problem of the coefficients  $b_i$  alone. Given the  $b_i$ , coefficients  $a_i$  are uniquely determined as solution of an (overdetermined) system of linear equations.

This approach reduces the dimension of the search space by half and improves numerical stability and accuracy. As a convex problem, the solution is unique and global.

To solve the nonlinear part, the function 1sqnonlin that uses the Levenberg-Marquard algorithm will be applied.

#### Value

mexpfit returns a list with the following elements:

- a0: the absolute term, 0 if const is false.
- a: linear coefficients.
- b: coefficient in the exponential functions.
- ssq: the sum of squares for the final fitting.
- iter: number of iterations resp. function calls.
- errmess: an error or info message.

#### Note

As the Jacobian for this expression is known, a more specialized approch would be possible, without using lsqnonlin; see the immoptibox of H. B. Nielsen, Techn. University of Denmark.

#### Author(s)

HwB email: <a href="mailto:</a> <a href="mailto:hwborchers@googlemail.com">hwborchers@googlemail.com</a>

#### References

Madsen, K., and H. B. Nielsen (2010). Introduction to Optimization and Data Fitting. Technical University of Denmark, Intitute of Computer Science and Mathematical Modelling.

Nielsen, H. B. (2000). Separable Nonlinear Least Squares. IMM, DTU, Report IMM-REP-2000-01. www.imm.dtu.dk/~hbn/publ/TR0001.ps

#### See Also

lsqsep, lsqnonlin

mldivide 201

#### **Examples**

```
Lanczos1 data (artificial data)
   f(x) = 0.0951 \times exp(-x) + 0.8607 \times exp(-3 \times x) + 1.5576 \times exp(-5 \times x)
x <- linspace(0, 1.15, 24)
y \leftarrow c(2.51340000, 2.04433337, 1.66840444, 1.36641802, 1.12323249, 0.92688972,
       0.76793386, 0.63887755, 0.53378353, 0.44793636, 0.37758479, 0.31973932,
        0.27201308, \ 0.23249655, \ 0.19965895, \ 0.17227041, \ 0.14934057, \ 0.13007002, 
       0.11381193, 0.10004156, 0.08833209, 0.07833544, 0.06976694, 0.06239313)
p0 < -c(-0.3, -5.5, -7.6)
mexpfit(x, y, p0, const = FALSE)
## $a0
## [1] 0
## $a
## [1] 0.09510431 0.86071171 1.55758398
## [1] -1.000022 -3.000028 -5.000009
## $ssa
## [1] 1.936163e-16
## $iter
## [1] 26
## $errmess
## [1] "Stopped by small gradient."
```

mldivide

Matlab backslash operator

#### **Description**

Emulate the Matlab backslash operator "\" through QR decomposition.

### Usage

```
mldivide(A, B, pinv = TRUE)
mrdivide(A, B, pinv = TRUE)
```

#### **Arguments**

A, B

Numerical or complex matrices; A and B must have the same number of rows (for mldivide) or the same number of columns (for mrdivide)

pinv

logical; shall SVD decomposition be used; default true.

#### Details

mldivide performs matrix left division (and mrdivide matrix right division). If A is scalar it performs element-wise division.

If A is square, mldivide is roughly the same as inv(A) %\*% B except it is computed in a different way — using QR decomposition.

202 mod, rem

If pinv = TRUE, the default, the SVD will be used as pinv(t(A)%\*%A)%\*%t(A)%\*%B to generate results similar to Matlab. Otherwise, qr. solve will be used.

If A is not square,  $x \leftarrow mldivide(A, b)$  returnes a least-squares solution that minimizes the length of the vector A \*\*\* x - b (which is equivalent to norm(A \*\*\* x - b, "F").

### Value

If A is an n-by-p matrix and B n-by-q, then the result of mldivide(A, B) is a p-by-q matrix (mldivide).

#### Note

mldivide(A, B) corresponds to A\B in Matlab notation.

#### **Examples**

```
# Solve a system of linear equations
A <- matrix(c(8,1,6, 3,5,7, 4,9,2), nrow = 3, ncol = 3, byrow = TRUE)
b <- c(1, 1, 1)
mldivide(A, b) # 0.066666667 0.06666667

A <- rbind(1:3, 4:6)
mldivide(A, c(1,1)) # -0.5 0 0.5 ,i.e. Matlab/Octave result
mldivide(A, c(1,1), pinv = FALSE) # -1 1 0 R qr.solve result</pre>
```

mod, rem

Integer Division

#### **Description**

Integer division functions and remainders

#### Usage

```
mod(n, m)
rem(n, m)
idivide(n, m, rounding = c("fix", "floor", "ceil", "round"))
```

## Arguments

```
n numeric vector (preferably of integers)
m must be a scalar integer (positive, zero, or negative)
rounding rounding mode.
```

Mode 203

### **Details**

mod(n, m) is the modulo operator and returns  $n \mod m$ . mod(n, 0) is n, and the result always has the same sign as m.

rem(n, m) is the same modulo operator and returns  $n \mod m$ . mod(n, 0) is NaN, and the result always has the same sign as n.

idivide(n, m) is integer division, with the same effect as n %/% m or using an optional rounding mode.

#### Value

a numeric (integer) value or vector/matrix.

#### Note

```
The following relation is fulfilled (for m != 0):

mod(n, m) = n - m * floor(n/m)
```

#### See Also

Binary R operators %/% and %%.

### **Examples**

```
mod(c(-5:5), 5)
rem(c(-5:5), 5)

idivide(c(-2, 2), 3, "fix")  # 0 0
idivide(c(-2, 2), 3, "floor")  # -1 0
idivide(c(-2, 2), 3, "ceil")  # 0 1
idivide(c(-2, 2), 3, "round")  # -1 1
```

Mode

Mode function (Matlab style)

### **Description**

Most frequent value in vector or matrix

# Usage

```
Mode(x)
```

#### **Arguments**

Real or complex vector or of factor levels.

204 moler

#### **Details**

Computes the 'sample mode', i.e. the most frequently occurring value in x.

Among values occurring equally frequently, Mode() chooses the smallest one (for a numeric vector), one with a smallest absolute value (for complex ones) or the first occurring value (for factor levels).

A matrix will be changed to a vector.

#### Value

One element from x and of the same type. The number of occurrences will not be returned.

#### Note

In Matlab/Octave an array dimension can be selected along which to find the mode value; this has not been realized here.

Shadows the R function mode that returns essentially the type of an object.

#### See Also

median

#### **Examples**

```
x <- round(rnorm(1000), 2)
Mode(x)</pre>
```

moler

Moler Matrix

### **Description**

Generate the Moler matrix of size  $n \times n$ . The Moler matrix is for testing eigenvalue computations.

### Usage

```
moler(n)
```

### **Arguments**

n

integer

#### **Details**

The Moler matrix for testing eigenvalue computations is a symmetric matrix with exactly one small eigenvalue.

#### Value

```
matrix of size n x n
```

movavg 205

#### See Also

```
wilkinson
```

### **Examples**

```
(a <- moler(10))
min(eig(a))</pre>
```

movavg

Moving Average Filters

### **Description**

Different types of moving average of a time series.

#### Usage

```
movavg(x, n, type=c("s", "t", "w", "m", "e", "r"))
```

### **Arguments**

```
x time series as numeric vector.

n backward window length.

type one of "s", "t", "w", "m", "e", or "r".
```

#### **Details**

Types of available moving averages are:

- s for "simple", it computes the simple moving average. n indicates the number of previous data points used with the current data point when calculating the moving average.
- t for "triangular", it computes the triangular moving average by calculating the first simple moving average with window width of ceil(n+1)/2; then it calculates a second simple moving average on the first moving average with the same window size.
- w for "weighted", it calculates the weighted moving average by supplying weights for each element in the moving window. Here the reduction of weights follows a linear trend.
- m for "modified", it calculates the modified moving average. The first modified moving average is calculated like a simple moving average. Subsequent values are calculated by adding the new value and subtracting the last average from the resulting sum.
- e for "exponential", it computes the exponentially weighted moving average. The exponential moving average is a weighted moving average that reduces influences by applying more weight to recent data points () reduction factor 2/(n+1); or
- r for "running", this is an exponential moving average with a reduction factor of 1/n [same as the modified average?].

206 movavg

#### Value

Vector the same length as time series x.

#### References

Matlab Techdoc

#### See Also

filter

```
## Not run:
abbshares <- scan(file="")
25.69 25.89 25.86 26.08 26.41 26.90 26.27 26.45 26.49 26.08 26.11 25.57 26.02
25.53 25.27 25.95 25.19 24.78 24.96 24.63 25.68 25.24 24.87 24.71 25.01 25.06
25.62 25.95 26.08 26.25 25.91 26.61 26.34 25.55 25.36 26.10 25.63 25.52 24.74
25.00 25.38 25.01 24.57 24.95 24.89 24.13 23.83 23.94 23.74 23.12 23.13 21.05
21.59 19.59 21.88 20.59 21.59 21.86 22.04 21.48 21.37 19.94 19.49 19.46 20.34
20.59 19.96 20.18 20.74 20.83 21.27 21.19 20.27 18.83 19.46 18.90 18.09 17.99
18.03 18.50 19.11 18.94 18.21 18.06 17.66 16.77 16.77 17.10 17.62 17.22 17.95
17.08 16.42 16.71 17.06 17.75 17.65 18.90 18.80 19.54 19.23 19.48 18.98 19.28
18.49 18.49 19.08 19.63 19.40 19.59 20.37 19.95 18.81 18.10 18.32 19.02 18.78
18.68 19.12 17.79 18.10 18.64 18.28 18.61 18.20 17.82 17.76 17.26 17.08 16.70
16.68 17.68 17.70 18.97 18.68 18.63 18.80 18.81 19.03 18.26 18.78 18.33 17.97
17.60 17.72 17.79 17.74 18.37 18.24 18.47 18.75 18.66 18.51 18.71 18.83 19.82
19.71 19.64 19.24 19.60 19.77 19.86 20.23 19.93 20.33 20.98 21.40 21.14 21.38
20.89 21.08 21.30 21.24 20.55 20.83 21.57 21.67 21.91 21.66 21.53 21.63 21.83
21.48 21.71 21.44 21.67 21.10 21.03 20.83 20.76 20.90 20.92 20.80 20.89 20.49
20.70 20.60 20.39 19.45 19.82 20.28 20.24 20.30 20.66 20.66 21.00 20.88 20.99
20.61 20.45 20.09 20.34 20.61 20.29 20.20 20.00 20.41 20.70 20.43 19.98 19.92
19.77 19.23 19.55 19.93 19.35 19.66 20.27 20.10 20.09 20.48 19.86 20.22 19.35
19.08 18.81 18.87 18.26 18.27 17.91 17.68 17.73 17.56 17.20 17.14 16.84 16.47
16.45 16.25 16.07
plot(abbshares, type = "1", col = 1, ylim = c(15, 30),
                main = "Types of moving averages", sub = "Mid 2011--Mid 2012",
                xlab = "Days", ylab = "ABB Shares Price (in USD)")
y <- movavg(abbshares, 50, "s"); lines(y, col = 2)</pre>
y <- movavg(abbshares, 50, "t"); lines(y, col = 3)</pre>
y <- movavg(abbshares, 50, "w"); lines(y, col = 4)</pre>
y <- movavg(abbshares, 50, "m"); lines(y, col = 5)
y <- movavg(abbshares, 50, "e"); lines(y, col = 6)</pre>
y <- movavg(abbshares, 50, "r"); lines(y, col = 7)</pre>
grid()
legend(120, 29, c("original data", "simple", "triangular", "weighted",
                                    "modified", "exponential", "running"),
                col = 1:7, lty = 1, lwd = 1, box.col = "gray", bg = "white")
## End(Not run)
```

muller 207

## Description

Muller's root finding method, similar to the secant method, using a parabola through three points for approximating the curve.

### Usage

```
muller(f, p0, p1, p2 = NULL, maxiter = 100, tol = 1e-10)
```

### **Arguments**

f	function whose root is to be found; function needs to be defined on the complex plain.
p0, p1, p2	three starting points, should enclose the assumed root.
tol	relative tolerance, change in successive iterates.
maxiter	maximum number of iterations.

#### **Details**

Generalizes the secant method by using parabolic interpolation between three points. This technique can be used for any root-finding problem, but is particularly useful for approximating the roots of polynomials, and for finding zeros of analytic functions in the complex plane.

### Value

```
List of root, fval, niter, and reltol.
```

#### Note

Muller's method is considered to be (a bit) more robust than Newton's.

#### References

Pseudo- and C code available from the 'Numerical Recipes'; pseudocode in the book 'Numerical Analysis' by Burden and Faires (2011).

### See Also

```
secant, newtonRaphson, newtonsys
```

208 nchoosek

#### **Examples**

```
muller(function(x) x^10 - 0.5, 0, 1) # root: 0.9330329915368074
f \leftarrow function(x) x^4 - 3*x^3 + x^2 + x + 1
p0 <- 0.5; p1 <- -0.5; p2 <- 0.0
muller(f, p0, p1, p2)
## $root
## [1] -0.3390928-0.4466301i
## ...
## Roots of complex functions:
fz \leftarrow function(z) \sin(z)^2 + sqrt(z) - \log(z)
muller(fz, 1, 1i, 1+1i)
## $root
## [1] 0.2555197+0.8948303i
## $fval
## [1] -4.440892e-16+0i
## $niter
## [1] 8
## $reltol
## [1] 3.656219e-13
```

nchoosek

Binomial Coefficients

# Description

Compute the Binomial coefficients.

#### Usage

```
nchoosek(n, k)
```

### **Arguments**

n, k

integers with k between 0 and n

#### **Details**

Alias for the corresponding R function choose.

### Value

```
integer, the Binomial coefficient (\frac{n}{k}).
```

#### Note

In Matlab/Octave, if n is a vector all combinations of k elements from vector n will be generated. Here, use the function combs instead.

ndims 209

### See Also

choose

### **Examples**

```
S <- sapply(0:6, function(k) nchoosek(6, k)) # 1 6 15 20 15 6 1
# Catalan numbers
catalan <- function(n) choose(2*n, n)/(n+1)
catalan(0:10)
# 1 1 2 5 14 42 132 429 1430 4862 16796
# Relations
n <- 10
sum((-1)^c(0:n) * sapply(0:n, function(k) nchoosek(n, k))) # 0</pre>
```

ndims

Number of Dimensions

# Description

Number of matrix or array dimensions.

#### Usage

ndims(x)

### **Arguments**

Х

a vector, matrix, array, or list

#### **Details**

Returns the number of dimensions as length(x).

A vector is seen as a matrix with one row, i.e. for a vector the number of dimensions is 2.

#### Value

the number of dimensions in the vector or array x.

### Note

The result will differ from Matlab when x is a character vector.

### See Also

size

210 nearest\_spd

### **Examples**

```
ndims(1:8)
ndims(array(1:8, c(2,2,2)))
```

nearest\_spd

Nearest Symmetric Positive-definite Matrix

# Description

Find nearest (in Frobenius norm) symmetric positive-definite matrix to A.

#### **Usage**

```
nearest_spd(A)
```

#### **Arguments**

Α

square numeric matrix.

#### **Details**

"The nearest symmetric positive semidefinite matrix in the Frobenius norm to an arbitrary real matrix A is shown to be (B + H)/2, where H is the symmetric polar factor of B=(A + A')/2." N. J. Highham

#### Value

Returns a matrix of the same size.

#### References

Nicholas J. Higham (1988). Computing a nearest symmetric positive semidefinite matrix. Linear Algebra and its Applications. Vol. 103, pp.103-118.

### See Also

```
rortho, procrustes
```

nelder\_mead 211

nelder_mead Nelder-Mead Minimization
--------------------------------------

### **Description**

An implementation of the Nelder-Mead algorithm for derivative-free optimization / function minimization.

### Usage

```
nelder_mead(x0, f, lb = NULL, ub = NULL, tol = 1e-10,

maxfeval = 20000, step = rep(1.0, length(x0)), ...)
```

#### **Arguments**

x0	starting vector.
f	nonlinear function to be minimized.
lb, ub	lower and upper of a bounded region.
tol	relative tolerance, to be used as stopping rule.
maxfeval	maximum number of function calls.
step	size and shape of initial simplex; relative magnitudes of its elements should reflect the units of the variables.
	additional arguments to be passed to the function.

### **Details**

Also called a 'simplex' method for finding the local minimum of a function of several variables. The method is a pattern search that compares function values at the vertices of the simplex. The process generates a sequence of simplices with ever reducing sizes.

'nelder\_mead()' can be used up to 20 dimensions (than 'tol' and 'maxfeval' need to be increased).

With upper and/or lower bounds, 'nelder\_mead()' applies a transformation of bounded to unbounded regions before utilizing Nelder-Mead. Of course, if the optimum is near to the boundary, results will not be as accurate as when the minimum is in the interior.

#### Value

List with following components:

xmin minimum solution found.fmin value of f at minimum.

nfeval number of iterations performed.

restarts number of restarts.

212 nelder\_mead

### Note

Original FORTRAN77 version by R O'Neill; MATLAB version by John Burkardt under LGPL license. Re-implemented in R by Hans W. Borchers. For another elaborate implementation of Nelder-Mead see the package 'dfoptim'.

#### References

Nelder, J., and R. Mead (1965). A simplex method for function minimization. Computer Journal, Volume 7, pp. 308-313.

O'Neill, R. (1971). Algorithm AS 47: Function Minimization Using a Simplex Procedure. Applied Statistics, Volume 20(3), pp. 338-345.

#### See Also

hooke\_jeeves

```
## Rosenbrock function
rosenbrock <- function(x) {</pre>
    n \leftarrow length(x)
    x1 <- x[2:n]
    x2 <- x[1:(n-1)]
    sum(100*(x1-x2^2)^2 + (1-x2)^2)
}
nelder_mead(c(0,0,0,0), rosenbrock)
# $xmin
# [1] 1 1 1 1
# $fmin
# [1] 8.802801e-25
# $nfeval
# [1] 678
# $restarts
# [1] 0
nelder_mead(c(0,0,0,0), rosenbrock, rep(-0.5, 4), rep(0.5, 4))
# [1] 0.50000000 0.26221321 0.07797600 0.00608026
# $fmin
# [1] 1.667875
# $nfeval
# [1] 1501
# $restarts
# [1] 3
```

neville 213

neville

Neville's Method

### **Description**

Neville's's method of polynomial interpolation.

# Usage

```
neville(x, y, xs)
```

### **Arguments**

```
x, yx-, y-coordinates of data points defining the polynomial.xssingle point to be interpolated.
```

#### **Details**

Straightforward implementation of Neville's method; not yet vectorized.

# Value

Interpolated value at xs of the polynomial defined by x, y.

#### References

Each textbook on numerical analysis.

### See Also

```
newtonInterp, barylag
```

```
p <- Poly(c(1, 2, 3))
fp <- function(x) polyval(p, x)

x <- 0:4; y <- fp(x)
xx <- linspace(0, 4, 51)
yy <- numeric(51)
for (i in 1:51) yy[i] <- neville(x, y, xx[i])

## Not run:
ezplot(fp, 0, 4)
points(xx, yy)
## End(Not run)</pre>
```

214 newmark

newmark	Newmark Method
---------	----------------

### **Description**

Newmark's is a method to solve higher-order differential equations without passing through the equivalent first-order system. It generalizes the so-called 'leap-frog' method. Here it is restricted to second-order equations.

#### Usage

```
newmark(f, t0, t1, y0, ..., N = 100, zeta = 0.25, theta = 0.5)
```

### **Arguments**

f	function in the differential equation $y'' = f(x, y, y')$ ; defined as a function $R \times R^2 \to R$ .
t0, t1	start and end points of the interval.
y0	starting values as row or column vector; $y0$ needs to be a vector of length 2, the first component representing $y(t0)$ , the second $dy/dt(t0)$ .
N	number of steps.
zeta, theta	two non-negative real numbers.
	Additional parameters to be passed to the function.

#### **Details**

Solves second order differential equations using the Newmark method on an equispaced grid of N steps.

Function f must return a vector, whose elements hold the evaluation of f(t,y), of the same dimension as y0. Each row in the solution array Y corresponds to a time returned in t.

The method is 'implicit' unless zeta=theta=0, second order if theta=1/2 and first order accurate if theta!=1/2. theta>=1/2 ensures stability. The condition set theta=1/2; zeta=1/4 (the defaults) is a popular approach that is unconditionally stable, but introduces oscillatory spurious solutions on long time intervals. (For these simulations it is preferable to use theta>1/2 and zeta>(theta+1/2)^(1/2).)

No attempt is made to catch any errors in the root finding functions.

### Value

List with components t for grid (or 'time') points between t0 and t1, and y an n-by-2 matrix with solution variables in columns, i.e. each row contains one time stamp.

#### Note

This is for demonstration purposes only; for real problems or applications please use ode23 or rk4sys.

newtonHorner 215

#### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

#### See Also

```
ode23, cranknic
```

## Examples

newtonHorner

Newton's Root Finding Method for Polynomials.

### **Description**

Finding roots of univariate polynomials.

#### **Usage**

```
newtonHorner(p, x0, maxiter = 50, tol = .Machine$double.eps^0.5)
```

#### **Arguments**

```
p Numeric vector representing a polynomial.

x0 starting value for newtonHorner().

maxiter maximum number of iterations; default 100.

tol absolute tolerance; default eps^(1/2)
```

#### **Details**

Similar to newtonRahson, except that the computation of the derivative is done through the Horner scheme in parallel with computing the value of the polynomial. This makes the algorithm significantly faster.

216 newtonInterp

#### Value

Return a list with components root, f.root, the function value at the found root, iter, the number of iterations done, and root, and the estimated precision estim.prec

The estimated precision is given as the difference to the last solution before stop.

#### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

#### See Also

newtonRaphson

### **Examples**

```
## Example: x^3 - 6 x^2 + 11 x - 6 with roots 1, 2, 3
p <- c(1, -6, 11, -6)
x0 <- 0
while (length(p) > 1) {
    N <- newtonHorner(p, x0)
    if (!is.null(N$root)) {
        cat("x0 =", N$root, "\n")
        p <- N$deflate
    } else {
        break
    }
}
## Try: p <- Poly(c(1:20))</pre>
```

newtonInterp

Lagrange and Newtons Interpolation

### **Description**

Lagrange's and Newton's method of polynomial interpolation.

### Usage

```
newtonInterp(x, y, xs = c())
lagrangeInterp(x, y, xs)
```

### **Arguments**

```
x, y x-, y-coordinates of data points defining the polynomial.
xs either empty, or a vector of points to be interpolated.
```

newtonRaphson 217

### **Details**

Straightforward implementation of Lagrange's Newton's method (vectorized in xs).

#### Value

A vector of values at xs of the polynomial defined by x, y.

#### References

Each textbook on numerical analysis.

#### See Also

```
neville, barylag
```

# **Examples**

```
p <- Poly(c(1, 2, 3))
fp <- function(x) polyval(p, x)

x <- 0:4; y <- fp(x)
xx <- linspace(0, 4, 51)
yy <- lagrangeInterp(x, y, xx)
yy <- newtonInterp(x, y, xx)
## Not run:
ezplot(fp, 0, 4)
points(xx, yy)
## End(Not run)</pre>
```

newtonRaphson

Rootfinding through Newton-Raphson or Secant.

# Description

Finding roots of univariate functions.

# Usage

218 newtonRaphson

# **Arguments**

fun	Function or its name as a string.
x0	starting value for newtonRaphson().
dfun	A function to compute the derivative of f. If NULL, a numeric derivative will be computed.
а	For secant one of the two starting values.
b	Another starting value.
maxiter	maximum number of iterations; default 100.
tol	absolute tolerance; default eps^(1/2)
	Additional arguments to be passed to f.

# **Details**

Well known root finding algorithms for real, univariate, continuous functions.

### Value

Return a list with components root, f.root, the function value at the found root, iter, the number of iterations done, and root, and the estimated precision estim.prec

For both methods the estimated precision is given as the difference to the last solution before stop; this may be misleading.

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

# See Also

newtonHorner

```
# Legendre polynomial of degree 5 lp5 <- c(63, 0, -70, 0, 15, 0)/8 f <- function(x) polyval(lp5, x) newton(f, 1.0)  # 0.9061798459 correct to 10 decimals in 5 iterations secant(f, 0.9, 1)  # 0.9061798459 correct to 10 decimals in 5 iterations
```

newtonsys 219

newtonsys	Newton Method for Nonlinear Systems

# Description

Newton's method applied to multivariate nonlinear functions.

# Usage

### **Arguments**

Ffun	m functions of n variables.
Jfun	Function returning a square n-by-n matrix (of partial derivatives) or NULL, the default.
x0	Numeric vector of length n.
maxiter	Maximum number of iterations.
tol	Tolerance, relative accuracy.
	Additional parameters to be passed to f.

#### **Details**

Solves the system of equations applying Newton's method with the univariate derivative replaced by the Jacobian.

# Value

List with components: zero the root found so far, fnorm the square root of sum of squares of the values of f, and iter the number of iterations needed.

### Note

TODO: better error checking, e.g. when the Jacobian is not invertible.

# References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

newtonRaphson, broyden

220 nextpow2

### **Examples**

```
## Example from Quarteroni & Saleri
F1 <- function(x) c(x[1]^2 + x[2]^2 - 1, sin(pi*x[1]/2) + x[2]^3)
newtonsys(F1, x0 = c(1, 1)) # zero: 0.4760958 -0.8793934
## Find the roots of the complex function \sin(z)^2 + \operatorname{sqrt}(z) - \log(z)
F2 <- function(x) {
    z <- x[1] + x[2]*1i
    fz \leftarrow \sin(z)^2 + \operatorname{sqrt}(z) - \log(z)
    c(Re(fz), Im(fz))
newtonsys(F2, c(1, 1))
# $zero 0.2555197 0.8948303 , i.e. z0 = 0.2555 + 0.8948i
# $fnorm 2.220446e-16
# $niter 8
## Two more problematic examples
F3 <- function(x)
        c(2*x[1] - x[2] - exp(-x[1]), -x[1] + 2*x[2] - exp(-x[2]))
newtonsys(F3, c(0, 0))
# $zero 0.5671433 0.5671433
# $fnorm 0
# $niter 4
## Not run:
F4 <- function(x) # Dennis Schnabel
        c(x[1]^2 + x[2]^2 - 2, exp(x[1] - 1) + x[2]^3 - 2)
newtonsys(F4, c(2.0, 0.5))
# will result in an error ``missing value in ... err<tol && niter<maxiter''</pre>
## End(Not run)
```

nextpow2

Next Power of 2

### **Description**

Smallest power of 2 greater than the argument.

# Usage

```
nextpow2(x)
```

# **Arguments**

Χ

numeric scalar, vector, or matrix

#### **Details**

Computes the smalest integer n such that  $abs(x) \le 2^n$ . IF x is a vector or matrix, returns the result component-wise. For negative or complex values, the absolute value will be taken.

nile 221

### Value

```
an integer n such that x \leq 2^n.
```

#### See Also

pow2

# **Examples**

```
nextpow2(10) #=> 4
nextpow2(1:10) #=> 0 1 2 2 3 3 3 3 4 4
nextpow2(-2^10) #=> 10
nextpow2(.Machine$double.eps) #=> -52
```

nile

Nile overflow data

# Description

Nile overflow data 1871–1984, gathered mostly by H. E. Hurst.

# Usage

```
data("nile")
```

### **Format**

A data frame with 114 years of observations during the months Jan to Dec.

### **Details**

Monthly flow data taken at the Dongola measurement station just upstream from the high dam at Aswan.

### Source

```
https://raw.githubusercontent.com/LCAV/SignalsOfTheDay/master/Day%203/FloodsOfTheNile_data.txt
```

# References

R. Weron (2001). Estimating long range dependence: finite sample properties and confidence intervals. arXiv: http://arxiv.org/pdf/cond-mat/0103510v2.pdf.

222 nnz

### **Examples**

```
data(nile)
                               # loads "nile" data frame
## Not run:
nile_dt <- nile[, 2:13]</pre>
                               # erase the "years" column
# plot all years in one figure
plot(ts(nile_dt), plot.type="single")
# merge all years in one time series
nile_ts \leftarrow ts(c(t(nile[, 2:13])), frequency = 12, start = c(1871, 1))
# aggregated flow per year
nile_flow <- apply(nile_dt, 1, sum)</pre>
plot(ts(nile_flow, frequency = 1, start = 1871) / 1000,
    col = "darkblue", lwd = 2.0,
    main = "Nile flows 1871 - 1984", ylab = "Flow / 1000")
grid()
# Hurst exponent of yearly Nile flow
hurstexp(nile_flow)
# Simple R/S Hurst estimation: 0.7348662
# Corrected R over S Hurst exponent: 1.041862
# Empirical Hurst exponent: 0.6975531
# Corrected empirical Hurst exponent: 0.7136607
# Theoretical Hurst exponent: 0.5244148
## End(Not run)
```

nnz

Nonzero Elements

### **Description**

Number of non-zero elements.

# Usage

nnz(x)

# Arguments

Χ

a numeric or complex vector or matrix.

#### Value

the number of non-zero elements of x.

Norm 223

### See Also

find

# **Examples**

```
nnz(diag(10))
```

Norm

Vector Norm

# **Description**

The Norm function calculates several different types of vector norms for x, depending on the argument p.

### Usage

```
Norm(x, p = 2)
```

# **Arguments**

x Numeric vector; matrices not allowed.

p Numeric scalar or Inf, -Inf; default is 2

### **Details**

Norm returns a scalar that gives some measure of the magnitude of the elements of x. It is called the p-norm for values  $-Inf \le p \le Inf$ , defining Hilbert spaces on  $R^n$ .

```
Norm(x) is the Euclidean length of a vecor x; same as Norm(x, 2).

Norm(x, p) for finite p is defined as sum(abs(A)^p)^(1/p).

Norm(x, Inf) returns max(abs(x)), while Norm(x, -Inf) returns min(abs(x)).
```

### Value

Numeric scalar (or Inf), or NA if an element of x is NA.

#### Note

In Matlab/Octave this is called norm; R's norm function norm(x, "F") ('Frobenius Norm') is the same as Norm(x).

#### See Also

norm of a matrix

224 normest

### **Examples**

normest

Estimated Matrix Norm

# Description

Estimate the 2-norm of a real (or complex-valued) matrix. 2-norm is also the maximum absolute eigenvalue of M, computed here using the power method.

# Usage

```
normest(M, maxiter = 100, tol = .Machine$double.eps^(1/2))
```

### **Arguments**

M Numeric matrix; vectors will be considered as column vectors.

maxiter Maximum number of iterations allowed; default: 100.

tol Tolerance used for stopping the iteration.

#### **Details**

Estimate the 2-norm of the matrix M, typically used for large or sparse matrices, where the cost of calculating the norm (A) is prohibitive and an approximation to the 2-norm is acceptable.

Theoretically, the 2-norm of a matrix M is defined as

$$||M||_2=\maxrac{||M*x||_2}{||x||_2} ext{ for all } x
eq 0$$

where  $||.||_2$  is the Euclidean/Frobenius norm.

### Value

2-norm of the matrix as a positive real number.

### Note

If feasible, an accurate value of the 2-norm would simply be calculated as the maximum of the singular values (which are all positive):

```
max(svd(M)$d)
```

nthroot 225

### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Philadelphia.

#### See Also

```
cond, svd
```

# **Examples**

```
normest(magic(5)) == max(svd(magic(5))$d) # TRUE
normest(magic(100)) # 500050
```

nthroot

Real nth Root

# Description

Compute the real n-th root of real numbers.

### Usage

```
nthroot(x, n)
```

# Arguments

- x numeric vector or matrix
- n positive integer specifying the exponent 1/n.

### **Details**

Computes the n-th root real numbers of a numeric vector x, while  $x^{(1/n)}$  will return NaN for negative numbers, even in case n is odd. If some numbers in x are negative, n must be odd. (This is different in *Octave*)

### Value

Returns a numeric vector of solutions to  $x^{1/n}$ .

### See Also

sqrt

```
nthroot(c(1, -2, 3), 3) \#=> 1.000000 -1.259921 1.442250 (-2)^(1/3) \#=> NaN
```

226 nullspace

nullspace

Kernel or Nullspace

# Description

Kernel of the linear map defined by matrix M.

### Usage

```
nullspace(M)
null(M)
```

#### **Arguments**

М

Numeric matrix; vectors will be considered as column vectors.

### **Details**

The kernel (aka null space/nullspace) of a matrix M is the set of all vectors x for which Ax=0. It is computed from the QR-decomposition of the matrix.

null is simply an alias for nullspace – and the Matlab name.

#### Value

If M is an n-by-m (operating from left on m-dimensional column vectors), then N=nullspace(M) is a m-by-k matrix whose columns define a (linearly independent) basis of the k-dimensional kernel in R^m.

If the kernel is only the null vector (0 0 ... 0), then NULL will be returned.

As the rank of a matrix is also the dimension of its image, the following relation is true:

```
m = dim(nullspace(M)) + rank(M)
```

### Note

The image of M can be retrieved from orth().

#### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Philadelphia.

### See Also

```
Rank, orth, MASS:: Null
```

numderiv 227

### **Examples**

```
M <- matrix(1:12, 3, 4)
Rank(M)
N <- nullspace(M)
            [,1]
                        [,2]
                                  [,3]
# [1,] 0.4082483 -0.8164966 0.4082483
M1 \leftarrow matrix(1:6, 2, 3) \# of rank 2
M2 \leftarrow t(M1)
nullspace(M1)
                          # corresponds to 1 -2 1
nullspace(M2)
                          # NULL, i.e. 0 0
M <- magic(5)
                         #=> 5
Rank(M)
nullspace(M)
                          #=> NULL, i.e. 0 0 0 0 0
```

numderiv

Richardson's Numerical Derivative

### **Description**

Richardson's method applied to the computation of the numerical derivative.

### Usage

```
numderiv(f, x0, maxiter = 16, h = 1/2, ..., tol = .Machine$double.eps)
numdiff(f, x, maxiter = 16, h = 1/2, ..., tol = .Machine$double.eps)
```

### **Arguments**

f function to be differentiated.

x0, x point(s) at which the derivative is to be computed.

maxiter maximum number of iterations.

h starting step size, should be the default h=0.5.

tol relative tolerance.

... variables to be passed to function f.

#### **Details**

numderiv returns the derivative of f at x0, where x0 must be a single scalar in the domain of the function

numdiff is a vectorized form of numderiv such that the derivatives will be returned at all points of the vector x.

228 numel

### Value

Numeric scalar or vector of approximated derivatives.

### Note

See grad in the 'numDeriv' package for another implementation of Richardson's method in the context of numerical differentiation.

# References

Mathews, J. H., and K. D. Fink (1999). Numerical Methods Using Matlab. Third Edition, Prentice Hall.

#### See Also

```
fderiv, complexstep
```

# **Examples**

```
# Differentiate an anti-derivative function
f <- function(x) sin(x)*sqrt(1+sin(x))</pre>
F <- function(x)
        integrate(f, 0, x, rel.tol = 1e-12)$value
x0 <- 1
dF0 <- numderiv(F, x0, tol = 6.5e-15) #=> 1.141882942715462
f(x0)
                                         #
                                            1.141882942715464 true value
# fderiv(F, x0)
                                         #
                                            1.141882942704476
# numDeriv::grad(F, x0)
                                            1.141882942705797
# Compare over a whole period
x \leftarrow seq(0, 2*pi, length.out = 11)
\max(abs(numdiff(sin, x) - cos(x)))
                                           #=> 3.44e-15
\# \max(abs(numDeriv::grad(sin, x) - cos(x))) \# 7.70e-12
# Example from complex step
f \leftarrow function(x) \exp(x) / sqrt(sin(x)^3 + cos(x)^3)
x0 <- 1.5
numderiv(f, x0)
                                          # 4.05342789389876, error 0.5e-12
                                             4.053427893898621... true value
```

numel

Number of Elements

# **Description**

Number of elements in a vector, matrix, or array.

ode23 229

### Usage

```
numel(x)
```

# Arguments

Х

a vector, matrix, array or list

#### Value

the number of elements of a.

#### See Also

size

# **Examples**

```
numel(c(1:12))
numel(matrix(1:12, 3, 4))
```

ode23

Non-stiff (and stiff) ODE solvers

# **Description**

Runge-Kutta (2, 3)-method with variable step size, resp. (4,5)-method with Dormand-Price coefficients, or (7,8)-pairs with Fehlberg coefficients. The function f(t, y) has to return the derivative as a column vector.

# Usage

### **Arguments**

```
f function in the differential equation y'=f(x,y); defined as a function R\times R^m\to R^m, where m is the number of equations. t0, tfinal start and end points of the interval.  
y0 starting values as column vector; for m equations u0 needs to be a vector of length m.
```

230 ode23

jac jacobian of f as a function of x alone; if not specified, a finite difference approx-

imation will be used.

rtol, atol relative and absolute tolerance.

hmax maximal step size, default is (tfinal - t0)/10.

... Additional parameters to be passed to the function.

#### **Details**

ode23 is an integration method for systems of ordinary differential equations using second and third order Runge-Kutta-Fehlberg formulas with automatic step-size.

ode23s can be used to solve a stiff system of ordinary differential equations, based on a modified Rosenbrock triple method of order (2,3); See section 4.1 in [Shampine and Reichelt].

ode45 implements Dormand-Prince (4,5) pair that minimizes the local truncation error in the 5thorder estimate which is what is used to step forward (local extrapolation). Generally it produces more accurate results and costs roughly the same computationally.

ode78 implements Fehlberg's (7,8) pair and is a 7th-order accurate integrator therefore the local error normally expected is  $O(h^8)$ . However, because this particular implementation uses the 8th-order estimate for xout (i.e. local extrapolation) moving forward with the 8th-order estimate will yield errors on the order of  $O(h^9)$ . It requires 13 function evaluations per integration step.

#### Value

List with components t for grid (or 'time') points between t0 and tfinal, and y an n-by-m matrix with solution variables in columns, i.e. each row contains one time stamp.

#### Note

Copyright (c) 2004 C. Moler for the Matlab textbook version ode23tx.

#### References

Ascher, U. M., and L. R. Petzold (1998). Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations. SIAM.

L.F. Shampine and M.W. Reichelt (1997). The MATLAB ODE Suite. SIAM Journal on Scientific Computing, Vol. 18, pp. 1-22.

Moler, C. (2004). Numerical Computing with Matlab. Revised Reprint, SIAM. http://www.mathworks.com/moler/chapters.html.

https://sites.google.com/site/comperem/home/ode\_solvers

### See Also

rk4sys, deval

ode23 231

```
## Example1: Three-body problem
f <- function(t, y)</pre>
as.matrix(c(y[2]*y[3], -y[1]*y[3], 0.51*y[1]*y[2]))
y0 <- as.matrix(c(0, 1, 1))
t0 <- 0; tf <- 20
sol <- ode23(f, t0, tf, y0, rtol=1e-5, atol=1e-10)
## Not run:
matplot(sol\$t, sol\$y, type = "l", lty = 1, lwd = c(2, 1, 1),
        col = c("darkred", "darkblue", "darkgreen"),
        xlab = "Time [min]", ylab= "",
        main = "Three-body Problem")
grid()
## End(Not run)
## Example2: Van der Pol Equation
x'' + (x^2 - 1) x' + x = 0
f <- function(t, x)</pre>
        as.matrix(c(x[1] * (1 - x[2]^2) -x[2], x[1]))
t0 <- 0; tf <- 20
x0 <- as.matrix(c(0, 0.25))
sol \leftarrow ode23(f, t0, tf, x0)
## Not run:
plot(c(0, 20), c(-3, 3), type = "n",
     xlab = "Time", ylab = "", main = "Van der Pol Equation")
lines(sol$t, sol$y[, 1], col = "blue")
lines(sol$t, sol$y[, 2], col = "darkgreen")
grid()
## End(Not run)
## Example3: Van der Pol as stiff equation
vdP \leftarrow function(t,y) \ as.matrix(c(y[2], 10*(1-y[1]^2)*y[2]-y[1]))
ajax <- function(t, y)</pre>
            matrix(c(0, 1, -20*y[1]*y[2]-1, 10*(1-y[1]^2)), 2,2, byrow = TRUE)
sol <- ode23s(vdP, t0, tf, c(2, 0), jac = ajax, hmax = 1.0)
## Not run:
plot(sol$t, sol$y[, 1], col = "blue")
lines(sol$t, sol$y[, 1], col = "blue")
lines(solt, solt, solt, col = "red", lwd = 2)
grid()
## End(Not run)
## Example4: pendulum
m = 1.0; l = 1.0 # [kg] resp. [m]
g = 9.81; b = 0.7 # [m/s^2] resp. [N s/m]
fp = function(t, x)
        c( x[2] , 1/(1/3*m*1^2)*(-b*x[2]-m*g*1/2*sin(x[1])) )
t0 <- 0.0; tf <- 5.0; hmax = 0.1
y0 = c(30*pi/180, 0.0)
sol = ode45(fp, t0, tf, y0, hmax = 0.1)
## Not run:
matplot(sol$t, sol$y, type = "1", lty = 1)
```

232 odregress

```
grid()
## End(Not run)

## Example: enforced pendulum
g <- 9.81
L <- 1.0; Y <- 0.25; w <- 2.5
f <- function(t, y) {
    as.matrix(c(y[2], -g/L * sin(y[1]) + w^2/L * Y * cos(y[1]) * sin(w*t)))
}
y0 <- as.matrix(c(0, 0))
sol <- ode78(f, 0.0, 60.0, y0, hmax = 0.05)
## Not run:
plot(sol$t, sol$y[, 1], type="1", col="blue")
grid()
## End(Not run)</pre>
```

odregress

Orthogonal Distance Regression

# **Description**

Orthogonal Distance Regression (ODR, a.k.a. total least squares) is a regression technique in which observational errors on both dependent and independent variables are taken into account.

#### Usage

```
odregress(x, y)
```

### **Arguments**

x matrix of independent variables.

y vector representing dependent variable.

### Details

The implementation used here is applying PCA resp. the singular value decomposition on the matrix of independent and dependent variables.

### Value

Returns list with components coeff linear coefficients and intercept term, ssq sum of squares of orthogonal distances to the linear line or hyperplane, err the orthogonal distances, fitted the fitted values, resid the residuals, and normal the normal vector to the hyperplane.

### Note

The "geometric mean" regression not implemented because questionable.

odregress 233

### References

Golub, G.H., and C.F. Van Loan (1980). An analysis of the total least squares problem. Numerical Analysis, Vol. 17, pp. 883-893.

http://www.cs.cornell.edu/cv/ResearchPDF/Analysis.total.least.squares.prob.pdf

See ODRPACK or ODRPACK95 (TOMS Algorithm 676).

URL: http://docs.scipy.org/doc/external/odr ams.pdf

URL: http://semi.vt.edu/presentations/SEMI-March05\_Watson.pdf

#### See Also

1m

```
# Example in one dimension
x \leftarrow c(1.0, 0.6, 1.2, 1.4, 0.2)
y \leftarrow c(0.5, 0.3, 0.7, 1.0, 0.2)
odr <- odregress(x, y)
( cc <- odr$coeff )</pre>
# [1] 0.65145762 -0.03328271
lm(y \sim x)
# Coefficients:
# (Intercept)
                          Х
     -0.01379
               0.62931
# Prediction
xnew <- seq(0, 1.5, by = 0.25)
( ynew <- cbind(xnew, 1) %*% cc )
## Not run:
plot(x, y, xlim=c(0, 1.5), ylim=c(0, 1.2), main="Orthogonal Regression")
abline(lm(y \sim x), col="blue")
lines(c(0, 1.5), cc[1]*c(0, 1.5) + cc[2], col="red")
points(xnew, ynew, col = "red")
grid()
## End(Not run)
# Example in two dimensions
x \leftarrow cbind(c(0.92, 0.89, 0.85, 0.05, 0.62, 0.55, 0.02, 0.73, 0.77, 0.57),
           c(0.66, 0.47, 0.40, 0.23, 0.17, 0.09, 0.92, 0.06, 0.09, 0.60))
y <- x %*% c(0.5, 1.5) + 1
odr <- odregress(x, y); odr
# $coeff
# [1] 0.5 1.5 1.0
# $ssq
# [1] 1.473336e-31
y \leftarrow y + rep(c(0.1, -0.1), 5)
odr <- odregress(x, y); odr
# $coeff
# [1] 0.5921823 1.6750269 0.8803822
```

234 orth

orth

Range Space

# **Description**

Range space or image of a matrix.

### Usage

orth(M)

# Arguments

Μ

Numeric matrix; vectors will be considered as column vectors.

#### **Details**

B=orth(A) returns an orthonormal basis for the range of A. The columns of B span the same space as the columns of A, and the columns of B are orthogonal to each other.

The number of columns of B is the rank of A.

# Value

Matrix of orthogonal columns, spanning the image of M.

# References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Philadelphia.

# See Also

nullspace

```
M <- matrix(1:12, 3, 4)
Rank(M)  #=> 2
orth(M)
```

pade 235

pade	Pade Approximation	

# **Description**

A Pade approximation is a rational function (of a specified order) whose power series expansion agrees with a given function and its derivatives to the highest possible order.

# Usage

```
pade(p1, p2 = c(1), d1 = 5, d2 = 5)
```

#### **Arguments**

p1	polynomial representing or approximating the function, preferably the Taylor series of the function around some point.
p2	if present, the function is given as p1/p2.
d1	the degree of the numerator of the rational function.
d2	the degree of the denominator of the rational function.

#### **Details**

The relationship between the coefficients of p1 (and p2) and r1 and r2 is determined by a system of linear equations. The system is then solved by applying the pseudo-inverse pinv for for the left-hand matrix.

### Value

List with components r1 and r2 for the numerator and denominator polynomials, i.e. r1/r2 is the rational approximation sought.

#### Note

In general, errors for Pade approximations are smallest when the degrees of numerator and denominator are the same or when the degree of the numerator is one larger than that of the denominator.

### References

Press, W. H., S. A. Teukolsky, W. T Vetterling, and B. P. Flannery (2007). Numerical Recipes: The Art of Numerical Computing. Third Edition, Cambridge University Press, New York.

### See Also

```
taylor, ratInterp
```

236 pascal

# **Examples**

```
## Exponential function
p1 <- c(1/24, 1/6, 1/2, 1.0, 1.0)  # Taylor series of exp(x) at x=0
R <- pade(p1); r1 <- R$r1; r2 <- R$r2
f1 <- function(x) polyval(r1, x) / polyval(r2, x)
## Not run:
xs <- seq(-1, 1, length.out=51); ys1 <- exp(xs); ys2 <- f1(xs)
plot(xs, ys1, type = "1", col="blue")
lines(xs, ys2, col = "red")
grid()
## End(Not run)</pre>
```

pascal

Pascal Triangle

# Description

Pascal triangle in matrix format

# Usage

```
pascal(n, k = 0)
```

# Arguments

 $\begin{array}{ll} n & \quad \text{natural number} \\ k & \quad \text{natural number, } k <= n \end{array}$ 

# **Details**

Pascal triangle with k variations.

### Value

matrix representing the Pascal triangle

### See Also

nchoosek

```
pascal(5)
pascal(5, 1)
pascal(5, 2)
```

pchip 237

pchip

Hermitean Interpolation Polynomials

# Description

Piecewise Cubic Hermitean Interpolation Polynomials.

# Usage

```
pchip(xi, yi, x)
pchipfun(xi, yi)
```

# Arguments

xi, yi x- and y-coordinates of supporting nodes.x x-coordinates of interpolation points.

#### **Details**

pchip is a 'shape-preserving' piecewise cubic Hermite polynomial approach that apptempts to determine slopes such that function values do not overshoot data values. pchipfun is a wrapper around pchip and returns a function. Both pchip and the function returned by pchipfun are vectorized.

xi and yi must be vectors of the same length greater or equal 3 (for cubic interpolation to be possible), and xi must be sorted. pchip can be applied to points outside [min(xi), max(xi)], but the result does not make much sense outside this interval.

# Value

Values of interpolated data at points x.

### Author(s)

Copyright of the Matlab version from Cleve Moler in his book "Numerical Computing with Matlab", Chapter 3 on Interpolation. R Version by Hans W. Borchers, 2011.

#### References

Moler, C. (2004). Numerical Computing with Matlab. Revised Reprint, SIAM.

# See Also

```
interp1
```

238 peaks

# **Examples**

peaks

Peaks Function (Matlab Style)

# Description

An example functions in two variables, with peaks.

# Usage

```
peaks(v = 49, w)
```

# **Arguments**

```
v vector, whose length will be used, or a natural number.w another vector, will be used in meshgrid(x,y).
```

#### **Details**

peaks is a function of two variables, obtained by translating and scaling Gaussian distributions, which is useful for demonstrating three-dimensional plots.

### Value

Returns three matrices as a list with X, Y, and Z components, the first two being the result of the meshgrid function, and Z the application of the following function at the points of X and Y:

```
z \leftarrow 3 * (1-x)^2 * exp(-(x^2) - (y+1)^2) - 10 * (x/5 - x^3 - y^5) * exp(-x^2 - y^2) -
```

#### Note

The variant that peaks() will display the 3-dim. graph as in Matlab is not yet implemented.

perms 239

# See Also

```
meshgrid
```

# **Examples**

```
peaks(3)
## Not run:
P <- peaks()
x <- P$X[1,]; y <- P$Y[, 1]
persp(x, y, P$Z)
## End(Not run)</pre>
```

perms

Generate Permutations

# Description

Generates all permutations of a vector a.

# Usage

```
perms(a)
```

# Arguments

а

numeric vector of some length n

# **Details**

If a is a vector of length n, generate all permutations of the elements in a as a matrix of size  $n! \times n$  where each row represents one permutation.

A matrix will be expanded as vector.

# Value

matrix of permutations of the elements of a

#### Note

```
Not feasible for length(a) > 10.
```

# See Also

randperm

240 piecewise

### **Examples**

```
perms(6)
perms(1:6)
perms(c(1, exp(1), pi))
```

piecewise

Piecewise Linear Function

# **Description**

Compute zeros and area of a piecewise linear function.

# Usage

```
piecewise(x, y, abs = FALSE)
```

# Arguments

x, y x- and y-coordinates of points defining the piecewise linear function

logical; shall the integral or the total area between the x-axis and the function be calculated

# **Details**

Compute zeros and integral resp. area of a piecewise linear function given by points with x and y as coordinates.

# Value

Returns a list with the integral or area as first element and the vector as all zeroes as second.

#### See Also

```
trapz
```

```
x \leftarrow c(0, 2, 3, 4, 5)

y \leftarrow c(2, -2, 0, -2, 0)

piecewise(x, y)

piecewise(x, y, abs=TRUE)
```

pinv 241

pinv

Pseudoinverse or Generalized Inverse

# **Description**

Computes the Moore-Penrose generalized inverse of a matrix.

# Usage

```
pinv(A, tol=.Machine$double.eps^(2/3))
```

# **Arguments**

A matrix

tol tolerance used for assuming an eigenvalue is zero.

### **Details**

Compute the generalized inverse B of a matrix A using the singular value decomposition svd(). This generalized invers is characterized by this equation: A %\*% B %\*% A == A

The pseudoinverse B solves the problem to minimize |Ax - b| by setting x = Bb

```
s <- svd(A)
D <- diag(s$d)
Dinv <- diag(1/s$d)
U <- s$u; V <- s$v
X = V Dinv t(U)</pre>
```

Thus B is computed as s\$v %\*% diag(1/s\$d) %\*% t(s\$u).

### Value

The pseudoinverse of matrix A.

# Note

The pseudoinverse or 'generalized inverse' is also provided by the function ginv() in package 'MASS'. It is included in a somewhat simplified way to be independent of that package.

#### References

Ben-Israel, A., and Th. N. E. Greville (2003). Generalized Inverses - Theory and Applications. Springer-Verlag, New York.

#### See Also

```
MASS::ginv
```

242 plotyy

### **Examples**

```
A <- matrix(c(7,6,4,8,10,11,12,9,3,5,1,2), 3, 4)
b <- apply(A, 1, sum) # 32 16 20 row sum
x <- pinv(A) %*% b
A %*% x #=> 32 16 20 as column vector
```

plotyy

Plotting Two y-Axes

# **Description**

Line plot with y-axes on both left and right side.

### Usage

# **Arguments**

```
x-coordinates for the curves
x1, x2
y1, y2
                   the y-values, with ordinates y1 left, y2 right.
gridp
                   logical; shall a grid be plotted.
box.col
                   color of surrounding box.
                   type of the curves, line or points (for both data).
type
lwd
                   line width (for both data).
lty
                   line type (for both data).
xlab, ylab
                   text below and on the left.
                   main title of the plot.
main
col.y1, col.y2 colors to be used for the lines or points.
                   additional plotting parameters.
```

#### **Details**

Plots y1 versus x1 with y-axis labeling on the left and plots y2 versus x2 with y-axis labeling on the right.

The x-values should not be too far appart. To exclude certain points, use NA values. Both curves will be line or point plots, and have the same line type and width.

#### Value

Generates a graph, no return values.

polar 243

### See Also

```
plotrix::twoord.plot
```

### **Examples**

```
## Not run:
x <- seq(0, 20, by = 0.01)
y1 <- 200*exp(-0.05*x)*sin(x)
y2 <- 0.8*exp(-0.5*x)*sin(10*x)

plotyy(x, y1, x, y2, main = "Two-ordinates Plot")
## End(Not run)</pre>
```

polar

Polar Coordinate Plot (Matlab Style)

# Description

The polar function accepts polar coordinates, plots them in a Cartesian plane, and draws the polar grid on the plane.

### Usage

```
polar(t, r, type="1",
      col = "blue", grcol = "darkgrey", bxcol = "black",
      main = "Polar Plot", add = FALSE, ...)
```

# **Arguments**

t, r vectors specifying angle and radius.
type type of the plot, lines, points, or no plotting.
col color of the graph.
grcol, bxcol color of grid anf box around the plot.
main plot title.
add logical; if true, the graph will be plotted into the coordinate system of an existing plot.
... plotting parameters to be passed to the points function.

### **Details**

polar (theta, rho) creates a polar coordinate plot of the angle theta versus the radius rho. theta is the angle from the x-axis to the radius vector specified in radians; rho is the length of the radius vector.

Poly Poly

# Value

Generates a plot; no returns.

# **Examples**

```
## Not run:
t <- deg2rad(seq(0, 360, by = 2))
polar(t, cos(2*t), bxcol = "white", main = "Sine and Cosine")
polar(t, sin(2*t), col = "red", add = TRUE)
## End(Not run)</pre>
```

Poly

Define Polynomial by Roots

# **Description**

Define a polynomial by its roots.

# Usage

```
Poly(x)
```

# **Arguments**

Х

vector or square matrix

# **Details**

Computes the characteristic polynomial of an (n x n)-Matrix.

If x is a vector, Poly(x) is the vector of coefficients of the polynomial whose roots are the elements of x.

# Value

Vector representing a polynomial.

### Note

In Matlab/Octave this function is called poly().

### See Also

```
polyval, roots
```

```
Poly(c(1, -1, 1i, -1i)) # Solves x^4 -1 = 0
# Wilkinson's example:
roots(Poly(1:20))
```

poly2str 245

poly2str

Print Polynomial

# Description

Print polynomial as a character string.

# Usage

```
poly2str(p, svar = "x", smul = "*", d = options("digits")$digits)
```

# **Arguments**

p numeric vector representing a polynomial svar character representing the unknown, default x. smul multiplication symbol, default \*.

d significant digits, default options("digits").

### **Details**

Simple string manipulation.

### Value

Returns the usual string representing a polynomial in mathematics.

# **Examples**

```
poly2str(c(0))
poly2str(c(1, -1, 1, -1, 1))
poly2str(c(0, 1e-6, 1e6), d = 2)
```

polyadd

Adding Polynomials

# Description

Add two polynomials given as vectors.

# Usage

```
polyadd(p, q)
```

### **Arguments**

p, q Vectors representing two polynomials.

246 polyApprox

### **Details**

Polynomial addition realized simply by multiplying and summing up all the coefficients after extending vectors to the same length.

### Value

Vector representing a polynomial.

### Note

There is no such function in Matlab or Octave.

#### See Also

conv

# **Examples**

polyApprox

Polynomial Approximation

# **Description**

Generate a polynomial approximation.

### Usage

```
polyApprox(f, a, b, n, ...)
```

### **Arguments**

```
f function to be approximated.

a, b end points of the interval.

n degree of the polynomial.

further variables for function f.
```

### **Details**

Uses the Chebyshev coefficients to derive polynomial coefficients.

### Value

List with three components: the approximating polynomial, a function evaluating this polynomial, and the estimated precision over the given interval.

polyarea 247

# Note

The Chebyshev approximation is optimal in the sense of the  $L^1$  norm, but not as a solution of the *minimax* problem; for this, an application of the Remez algorithm is needed.

### References

Carothers, N. L. (1998). A Short Course on Approximation Theory. Bowling Green State University, URL: http://personal.bgsu.edu/~carother/Approx.html.

#### See Also

```
chebApprox, polyfit
```

# **Examples**

```
## Example
    Polynomial approximation for sin
polyApprox(sin, -pi, pi, 9)
# $p
# [1] 0.06549943 0.00000000 -0.58518036 0.00000000 2.54520983
# [7] 0.00000000 -5.16709776 0.00000000 3.14158037 0.00000000
# $f
# function (x)
# polyval(r, x)
# <environment: 0x1f978e8>
# $estim.prec
# [1] 1.151207e-05
## Not run:
f <- polyApprox(sin, -pi, pi, 9)$f</pre>
x \leftarrow seq(-pi, pi, length.out = 100)
y \leftarrow \sin(x) - f(x)
plot(x, y, type = "l", col = "blue")
grid()
## End(Not run)
```

polyarea

Area of a Polygon

# Description

Calculates the area and length of a polygon given by the vertices in the vectors x and y.

248 polyarea

### Usage

```
polyarea(x, y)
poly_length(x, y)
poly_center(x, y)
poly_crossings(L1, L2)
```

### **Arguments**

X	x-coordinates of the vertices defining the polygon
у	y-coordinates of the vertices
L1, L2	matrices of type 2xn with x- and y-coordinates.

# **Details**

polyarea calculates the area of a polygon defined by the vertices with coordinates x and y. Areas to the left of the vertices are positive, those to the right are counted negative.

The computation is based on the Gauss polygon area formula. The polygon automatically be closed, that is the last point need not be / should not be the same as the first.

If some points of self-intersection of the polygon line are not in the vertex set, the calculation will be inexact. The sum of all areas will be returned, parts that are circulated in the mathematically negative sense will be counted as negative in this sum.

If x, y are matrices of the same size, the areas of all polygons defined by corresponding columns are computed.

poly\_center calculates the center (of mass) of the figure defined by the polygon. Self-intersections should be avoided in this case. The mathematical orientation of the polygon does not have influence on the center coordinates.

poly\_length calculates the length of the polygon

poly\_crossings calculates the crossing points of two polygons given as matrices with x- and y-coordinates in the first and second row. Can be used for finding the crossing points of parametrizised curves.

#### Value

Area or length of the polygon resp. sum of the enclosed areas; or the coordinates of the center of gravity.

poly\_crossings returns a matrix with column names x and y representing the crossing points.

### See Also

```
trapz, arclength
```

polyarea 249

```
# Zu Chongzhi's calculation of pi (China, about 480 A.D.),
 # approximating the circle from inside by a regular 12288-polygon(!):
 phi <- seq(0, 2*pi, len=3*2^12+1)</pre>
 x < -\cos(phi)
 y <- sin(phi)
 pi_approx <- polyarea(x, y)</pre>
 print(pi_approx, digits=8)
                                 #=> 3.1415925 or 355/113
 poly_length(x, y)
                                  #=> 6.2831852 where 2*pi is 6.2831853
 x1 \leftarrow x + 0.5; y1 \leftarrow y + 0.5
 x2 \leftarrow rev(x1); y2 \leftarrow rev(y1)
 poly_center(x1, y1)
                                   #=> 0.5 0.5
                                  #=> 0.5 0.5
 poly_center(x2, y2)
 # A simple example
 L1 \leftarrow matrix(c(0, 0.5, 1, 1, 2,
                0, 1, 1, 0.5, 0), \text{ nrow} = 2, \text{ byrow} = \text{TRUE}
 L2 \leftarrow matrix(c(0.5, 0.75, 1.25, 1.25,
                0, 0.75, 0.75, 0), nrow = 2, byrow = TRUE)
 P <- poly_crossings(L1, L2)
 ##
           Х
 ## [1,] 1.00 0.750
 ## [2,] 1.25 0.375
## Not run:
 # Crossings of Logarithmic and Archimedian spirals
 # Logarithmic spiral
 a <- 1; b <- 0.1
 t <- seq(0, 5*pi, length.out = 200)
 xl \leftarrow a*exp(b*t)*cos(t) - 1
 yl <- a*exp(b*t)*sin(t)</pre>
 plot(x1, y1, type = "1", lwd = 2, col = "blue",
       xlim = c(-6, 3), ylim = c(-3, 4), xlab = "", ylab = "",
       main = "Intersecting Logarithmic and Archimedian spirals")
 grid()
 # Archimedian spiral
 a <- 0; b <- 0.25
 r \leftarrow a + b*t
 xa <- r * cos(t)
 ya \leftarrow r*sin(t)
 lines(xa, ya, type = "1", lwd = 2, col = "red")
 legend(-6.2, -1.0, c("Logarithmic", "Archimedian"),
         lwd = 2, col = c("blue", "red"), bg = "whitesmoke")
 L1 \leftarrow rbind(xl, yl)
 L2 <- rbind(xa, ya)
 P <- poly_crossings(L1, L2)
 points(P)
```

250 polyder

```
## End(Not run)
```

polyder

Derivative of Polynomial

# **Description**

Differentiate polynomials.

# Usage

```
polyder(p, q)
```

# Arguments

p polynomial p given as a vector

q polynomial p given as a vector

### **Details**

Calculates the derivative of polynomials and polynomial products.

polyder(p) returns the derivative of p while polyder(p, q) returns the derivative of the product of the polynomials p and q.

# Value

a vector representing a polynomial

# See Also

```
polyval, polyint
```

```
polyder(c(3, 6, 9), c(1, 2, 0)) # 12 36 42 18
```

polyfit 251

polyfit

Fitting by Polynomial

# **Description**

Polynomial curve fitting

# Usage

```
polyfit(x, y, n)
polyfit2(x, y, n = 1, p0 = NULL)
```

# **Arguments**

Χ	x-coordinates of points
у	y-coordinates of points
n	degree of the fitting polynomial
p0	Point $p0 = [x0, y0]$

# **Details**

polyfit finds the coefficients of a polynomial of degree n fitting the points given by their x, y coordinates in a least-squares sense.

polyfit2 finds a polynomial that fits the data in a least-squares sense, but also passes through y0 for x=x0.

In polyfit, if x, y are matrices of the same size, the coordinates are taken elementwise. Complex values are not allowed.

### Value

vector representing a polynomial

# See Also

```
poly, polyval
```

```
# Fitting the sine function by a polynomial
x <- seq(0, pi, length.out=25)
y <- sin(x)
p <- polyfit(x, y, 6)

## Not run:
    # Plot sin and fitted polynomial
plot(x, y, type="b")</pre>
```

252 polyint

```
yf <- polyval(p, x)
lines(x, yf, col="red")
grid()
## End(Not run)</pre>
```

polyint

Anti-derivative of Polynomial

# Description

Integrate polynomials.

# Usage

```
polyint(p, k)
```

# **Arguments**

p polynomial p given as a vector

k an integration constant

# **Details**

Calculates the integral, i.e. the antiderivative, of a polynomial and adds a constant of integration k if given, else 0.

# Value

a vector representing a polynomial

### See Also

```
polyval, polyder
```

```
polyint(c(1, 1, 1, 1, 1), 1)
```

polylog 253

polylog

Polylogarithm Function

## Description

Computes the n-based polylogarithm of z:  $Li_n(z)$ .

### Usage

```
polylog(z, n)
```

### **Arguments**

z real number or vector, all entries satisfying abs(z)<1.

n base of polylogarithm, integer greater or equal -4.

#### **Details**

The Polylogarithm is also known as Jonquiere's function. It is defined as

$$\sum_{k=1}^{\infty} z^k / k^n = z + z^2 / 2^n + \dots$$

The polylogarithm function arises, e.g., in Feynman diagram integrals. It also arises in the closed form of the integral of the Fermi-Dirac and the Bose-Einstein distributions.

The special cases n=2 and n=3 are called the dilogarithm and trilogarithm, respectively.

Approximation should be correct up to at least 5 digits for |z| > 0.55 and on the order of 10 digits for |z| <= 0.55.

### Value

Returns the function value (not vectorized).

#### Note

Based on some equations, see references. A Matlab implementation is available in the Matlab File Exchange.

## References

V. Bhagat, et al. (2003). On the evaluation of generalized BoseEinstein and FermiDirac integrals. Computer Physics Communications, Vol. 155, p.7.

254 polymul

### **Examples**

polymul

Multiplying Polynomials

## Description

Multiply two polynomials given as vectors.

### Usage

```
polymul(p, q)
```

### **Arguments**

p, q

Vectors representing two polynomials.

### **Details**

Polynomial multiplication realized simply by multiplying and summing up all the coefficients.

#### Value

Vector representing a polynomial.

#### Note

conv also realizes polynomial multiplication, through Fast Fourier Transformation, with the drawback that small imaginary parts may evolve.

#### See Also

```
conv, deconv
```

```
# Multiply x^2 + x + 1 with itself polymul(c(1, 1, 1), c(0, 1, 1, 1)) #=> 1 2 3 2 1
```

polypow 255

polypow

Polynomial Powers

## Description

Power of a polynomial.

# Usage

```
polypow(p, n)
```

## Arguments

p vector representing a polynomial.

n positive integer, the exponent.

### **Details**

Uses polymul to multiply the polynomial p n times with itself.

### Value

Vector representing a polynomial.

## Note

There is no such function in Matlab or Octave.

### See Also

```
polymul
```

256 polytrans

polytrans

Polynomial Transformation

# Description

Transform a polynomial.

## Usage

```
polytrans(p, q)
```

## Arguments

p, q vectors representing two polynomials.

### **Details**

Transforms polynomial p replacing occurences of x with another polynomial q in x.

### Value

Vector representing a polynomial.

#### Note

There is no such function in Matlab or Octave.

# See Also

```
polypow
```

polyval 257

polyval

Evaluating a Polynomial

## Description

Evaluate polynomial given as a numeric vector.

## Usage

```
polyval(p, x)
```

## **Arguments**

p vector representing a polynomial

x vector of values where to evaluate the polynomial

### **Details**

Evaluate the polynomial given by p at the values specified by the elements of x. If x is a matrix, the polynomial will be evaluated at each element and a matrix returned.

### Value

vector of values

### See Also

```
poly, roots
```

## **Examples**

```
# Evaluate 3 x^2 + 2 x + 1 at x = 5, 7, and 9 p = c(3, 2, 1); polyval(p, c(5, 7, 9)) # 86 162 262
```

pow2

Base 2 Power

# Description

Power with base 2.

### Usage

```
pow2(f, e)
```

258 ppfit

### **Arguments**

f numeric vector of factors

e numeric vector of exponents for base 2

#### **Details**

Computes the expression f \* 2^e, setting e to f and f to 1 in case e is missing. Complex values are only processed if e is missing.

#### Value

Returns a numeric vector computing  $f 2^e$ .

### See Also

```
nextpow2
```

### **Examples**

```
pow2(c(0, 1, 2, 3))  #=> 1 2 4 8

pow2(c(0, -1, 2, 3), c(0,1,-2,3))  #=> 0.0 -2.0 0.5 24.0

pow2(1i)  #=> 0.7692389+0.6389613i
```

ppfit

Piecewise Polynomial Fit

### **Description**

Piecewise linear or cubic fitting.

### Usage

```
ppfit(x, y, xi, method = c("linear", "cubic"))
```

## **Arguments**

x, y x-, y-coordinates of given points.

xi x-coordinates of the choosen support nodes.

method interpolation method, can be 'constant', 'linear', or 'cubic' (i.e., 'spline').

## **Details**

ppfit fits a piece-wise polynomial to the input independent and dependent variables,x and y, respectively. A weighted linear least squares solution is provided. The weighting vector w must be of the same size as the input variables.

ppval 259

### Value

Returns a pp (i.e., piecewise polynomial) structure.

#### Note

Following an idea of Copyright (c) 2012 Ben Abbott, Martin Helm for Octave.

#### See Also

```
mkpp, ppval
```

### **Examples**

```
x <- 0:39
y <- c( 8.8500, 32.0775, 74.7375, 107.6775, 132.0975, 156.6675,
       169.0650, 187.5375, 202.2575, 198.0750, 225.9600, 204.3550,
       233.8125, 204.5925, 232.3625, 204.7550, 220.1925, 199.5875,
       197.3025, 175.3050, 218.6325, 163.0775, 170.6625, 148.2850,
       154.5950, 135.4050, 138.8600, 125.6750, 118.8450, 99.2675,
       129.1675, 91.1925, 89.7000, 76.8825, 83.6625, 74.1950,
       73.9125, 55.8750, 59.8675, 48.1900)
xi <- linspace(0, 39, 8)
pplin <- ppfit(x, y, xi) # method = "linear"</pre>
ppcub <- ppfit(x, y, xi, method = "cubic")</pre>
## Not run:
plot(x, y, type = "b", main = "Piecewise polynomial approximation")
xs <- linspace(0, 39, 100)
yslin <- ppval(pplin, xs)</pre>
yscub <- ppval(ppcub, xs)</pre>
lines(xs, yscub, col="red",lwd = 2)
lines(xs, yslin, col="blue")
grid()
## End(Not run)
```

ppval

Piecewise Polynomial Structures

### Description

Make or evaluate a piecewise polynomial.

## Usage

```
mkpp(x, P)
ppval(pp, xx)
```

260 ppval

### **Arguments**

X	increasing vector of real numbers.
P	matrix containing the coefficients of polynomials in each row.
рр	a piecewise polynomial structure, generated by mkpp.
XX	numerical vector

#### **Details**

pp<-mkpp(x,P) builds a piecewise polynomial from its breaks x and coefficients P. x is a monotonically increasing vector of length L+1, and P is an L-by-k matrix where each row contains the coefficients of the polynomial of order k, from highest to lowest exponent, on the interval [x[i],x[i+1]).

ppval(pp,xx) returns the values of the piecewise polynomial pp at the entries of the vector xx. The first and last polynomial will be extended to the left resp. right of the interval [x[1],x[L+1]).

### Value

mkpp will return a piecewise polynomial structure, that is a list with components breaks=x, pieces=P, order=k and dim=1 for scalar-valued functions.

#### Note

Matlab allows to generate vector-valued piecewise polynomials. This may be included in later versions.

#### See Also

```
cubicspline
```

```
## Example: Linear interpolation of the sine function
xs <- linspace(0, pi, 10)
ys <- sin(xs)
P <- matrix(NA, nrow = 9, ncol = 2)
for (i in 1:9) {
    P[i, ] <- c((ys[i+1]-ys[i])/(xs[i+1]-xs[i]), ys[i])
}
ppsin <- mkpp(xs, P)

## Not run:
plot(xs, ys); grid()
x100 <- linspace(0, pi, 100)
lines(x100, sin(x100), col="darkgray")
ypp <- ppval(ppsin, x100)
lines(x100, ypp, col="red")

## End(Not run)</pre>
```

primes 261

primes

Prime Numbers

### Description

Generate a list of prime numbers less or equal n, resp. between n1 and n2.

### Usage

```
primes(n)
```

### **Arguments**

n

nonnegative integer greater than 1.

### **Details**

The list of prime numbers up to n is generated using the "sieve of Erasthostenes". This approach is reasonably fast, but may require a lot of main memory when n is large.

In double precision arithmetic integers are represented exactly only up to 2^53 - 1, therefore this is the maximal allowed value.

#### Value

vector of integers representing prime numbers

### See Also

```
isprime, factors
```

```
primes(1000)
## Not run:
## Appendix: Logarithmic Integrals and Prime Numbers (C.F.Gauss, 1846)
library('gsl')
# 'European' form of the logarithmic integral
Li <- function(x) expint_Ei(log(x)) - expint_Ei(log(2))
# No. of primes and logarithmic integral for 10<sup>i</sup>, i=1...12
i <- 1:12; N <- 10^i
# piN <- numeric(12)</pre>
# for (i in 1:12) piN[i] <- length(primes(10^i))</pre>
piN <- c(4, 25, 168, 1229, 9592, 78498, 664579,
         5761455, 50847534, 455052511, 4118054813, 37607912018)
cbind(i, piN, round(Li(N)), round((Li(N)-piN)/piN, 6))
# i
         pi(10^i)
                     Li(10^i) rel.err
```

262 procrustes

#				
#	1	4	5	0.280109
#	2	25	29	0.163239
#	3	168	177	0.050979
#	4	1229	1245	0.013094
#	5	9592	9629	0.003833
#	6	78498	78627	0.001637
#	7	664579	664917	0.000509
#	8	5761455	5762208	0.000131
#	9	50847534	50849234	0.000033
#	10	455052511	455055614	0.000007
#	11	4118054813	4118066400	0.000003
#	12	37607912018	37607950280	0.000001
#				
##	# En	d(Not run)		

procrustes

Solving the Procrustes Problem

### **Description**

procrustes solves for two matrices A and B the 'Procrustes Problem' of finding an orthogonal matrix Q such that A-B\*Q has the minimal Frobenius norm.

kabsch determines a best rotation of a given vector set into a second vector set by minimizing the weighted sum of squared deviations. The order of vectors is assumed fixed.

### Usage

```
procrustes(A, B)
kabsch(A, B, w = NULL)
```

### **Arguments**

A, B two numeric matrices of the same size.w weights, influence the distance of points

### **Details**

The function procrustes (A,B) uses the svd decomposition to find an orthogonal matrix Q such that A-B\*Q has a minimal Frobenius norm, where this norm for a matrix C is defined as sqrt(Trace(t(C)\*C)), or norm(C, 'F') in R.

Solving it with B=I means finding a nearest orthogonal matrix.

kabsch solves a similar problem and uses the Procrustes procedure for its purpose. Given two sets of points, represented as columns of the matrices A and B, it determines an orthogonal matrix U and a translation vector R such that U\*A+R-B is minimal.

procrustes 263

### Value

procrustes returns a list with components P, which is B\*Q, then Q, the orthogonal matrix, and d, the Frobenius norm of A-B\*Q.

kabsch returns a list with U the orthogonal matrix applied, R the translation vector, and d the least root mean square between U\*A+R and B.

#### Note

The kabsch function does not take into account scaling of the sets, but this could easily be integrated.

#### References

Golub, G. H., and Ch. F. van Loan (1996). Matrix Computations. 3rd Edition, The John Hopkins University Press, Baltimore London. [Sect. 12.4, p. 601]

Kabsch, W. (1976). A solution for the best rotation to relate two sets of vectors. Acta Cryst A, Vol. 32, p. 9223.

#### See Also

svd

```
## Procrustes
U <- rortho(5)
                                  # random orthogonal matrix
P <- procrustes(U, eye(5))
## Kabsch
P \leftarrow matrix(c(0, 1, 0, 0, 1, 1, 0, 1,
               0, 0, 1, 0, 1, 0, 1, 1,
               0, 0, 0, 1, 0, 1, 1, 1, nrow = 3, ncol = 8, byrow = TRUE)
R \leftarrow c(1, 1, 1)
phi <- pi/4
U <- matrix(c(1, 0, 0,
               0, cos(phi), -sin(phi),
               0, sin(phi), cos(phi)), nrow = 3, ncol = 3, byrow = TRUE)
Q <- U %*% P + R
K <- kabsch(P, Q)</pre>
\# KR == R \text{ and } KU \% P + c(KR) == Q
```

264 psi

psi

Psi (Polygamma) Function

### **Description**

Arbitrary order Polygamma function valid in the entire complex plane.

### Usage

```
psi(k, z)
```

### **Arguments**

k order of the polygamma function, whole number greater or equal 0.

z numeric complex number or vector.

#### **Details**

Computes the Polygamma function of arbitrary order, and valid in the entire complex plane. The polygamma function is defined as

$$\psi(n,z) = \frac{d^{n+1}}{dz^{n+1}} \log(\Gamma(z))$$

If n is 0 or absent then psi will be the Digamma function. If n=1,2,3,4,5 etc. then psi will be the tri-, tetra-, penta-, hexa-, hepta- etc. gamma function.

### Value

Returns a complex number or a vector of complex numbers.

qpspecial 265

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Special Quadratic Programming Solver

### **Description**

Solves a special Quadratic Programming problem.

### Usage

```
qpspecial(G, x, maxit = 100)
```

# Arguments

```
G m x n-matrix.
```

x column vector of length n, the initial (feasible) iterate; if not present (or requirements on x0 not met), x0 will be found.

maxit

maximum number of iterates allowed; default 100.

#### **Details**

Solves the QP problem

```
min q(x) = || G*x ||_2^2 = x'*(G'*G)*x
s.t. sum(x) = 1
and x >= 0
```

The problem corresponds to finding the smallest vector (2-norm) in the convex hull of the columns of G.

#### Value

Returns a list with the following components:

- x optimal point attaining optimal value;
- d = G\*x smallest vector in the convex hull;
- q optimal value found, = t(d) %\*% d;
- niter number of iterations used;
- info error number:
  - = 0: everything went well, q is optimal,
  - = 1: maxit reached and final x is feasible,
  - = 2: something went wrong.

## Note

x may be missing, same as if requirements are not met; may stop with an error if x is not feasible.

266 qrSolve

### Author(s)

Matlab code by Anders Skajaa, 2010, under GPL license (HANSO toolbox); converted to R by Abhirup Mallik and Hans W. Borchers, with permission.

### References

[Has to be found.]

## **Examples**

```
G \leftarrow matrix(c(0.31, 0.99, 0.54, 0.20,
              0.56, 0.97, 0.40, 0.38,
              0.81, 0.06, 0.44, 0.80), 3, 4, byrow =TRUE)
qpspecial(G)
# $x
                [,1]
# [1,] 1.383697e-07
# [2,] 5.221698e-09
# [3,] 8.648168e-01
# [4,] 1.351831e-01
# $d
            [,1]
# [1,] 0.4940377
# [2,] 0.3972964
# [3,] 0.4886660
# $q
# [1] 0.6407121
# $niter
# [1] 6
# $info
# [1] 0
```

qrSolve

LSE Solution

## Description

Systems of linear equations via QR decomposition.

### Usage

```
qrSolve(A, b)
```

quad 267

## **Arguments**

```
A numerical matrix with nrow(A)>=ncol(A).
b numerical vector with length(b) == nrow(A).
```

#### **Details**

Solves (overdetermined) systems of linear equations via QR decomposition.

#### Value

The solution of the system as vector.

### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Society for Industrial and Applied Mathematics, Philadelphia.

#### See Also

householder

### **Examples**

```
A <- matrix(c(0,-4,2, 6,-3,-2, 8,1,-1), 3, 3, byrow=TRUE)
b <- c(-2, -6, 7)
qrSolve(A, b)

## Solve an overdetermined linear system of equations
A <- matrix(c(1:8,7,4,2,3,4,2,2), ncol=3, byrow=TRUE)
b <- rep(6, 5)
x <- qrSolve(A, b)
qr.solve(A, rep(6, 5)); x</pre>
```

quad

Adaptive Simpson Quadrature

### **Description**

Adaptive quadrature of functions of one variable over a finite interval.

### Usage

```
quad(f, xa, xb, tol = .Machine$double.eps^0.5, trace = FALSE, ...)
```

268 quad

## Arguments

f	a one-dimensional function; needs to be vectorized.
xa	lower limit of integration; must be finite
xb	upper limit of integration; must be finite
tol	accuracy requested.
trace	logical; shall a trace be printed?
	additional arguments to be passed to f.

### **Details**

Realizes adaptive Simpson quadrature in R through recursive calls.

The function f needs to be vectorized though this could be changed easily. quad is not suitable for functions with singularities in the interval or at end points.

#### Value

A single numeric value, the computed integral.

#### Note

More modern adaptive methods based on Gauss-Kronrod or Clenshaw-Curtis quadrature are now generally preferred.

#### Author(s)

Copyright (c) 1998 Walter Gautschi for the Matlab version published as part of the referenced article. R implementation by Hans W Borchers 2011.

#### References

```
Gander, W. and W. Gautschi (2000). "Adaptive Quadrature — Revisited". BIT, Vol. 40, 2000, pp. 84-101. http://www.inf.ethz.ch/personal/gander
```

### See Also

```
integrate, quadl
```

quad2d 269

```
yy <- f(xx)
plot(xx, yy, type = 'l')
grid()
## End(Not run)</pre>
```

quad2d

2-d Gaussian Quadrature

### Description

Two-dimensional Gaussian Quadrature.

#### **Usage**

```
quad2d(f, xa, xb, ya, yb, n = 32, ...)
```

### **Arguments**

f	function of two variables; needs to be vectorized.
xa, ya	lower limits of integration; must be finite.
xb, yb	upper limits of integration; must be finite.
n	number of nodes used per direction.
	additional arguments to be passed to f.

### **Details**

Extends the Gaussian quadrature to two dimensions by computing two sets of nodes and weights (in x- and y-direction), evaluating the function on this grid and multiplying weights appropriately.

The function f needs to be vectorized in both variables such that f(X, Y) returns a matrix when X an Y are matrices (of the same size).

quad is not suitable for functions with singularities.

### Value

A single numerical value, the computed integral.

#### Note

The extension of Gaussian quadrature to two dimensions is obvious, but see also the example 'integral2d.m' at Nick Trefethens "10 digits 1 page", http://people.maths.ox.ac.uk/trefethen/ten\_digit\_algs.htm and Matlab code at http://people.maths.ox.ac.uk/trefethen/tda.html.

#### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

270 quadcc

### See Also

```
quad, cubature::adaptIntegrate
```

### **Examples**

quadcc

Adaptive Clenshaw-Curtis Quadrature

## Description

Adaptive Clenshaw-Curtis Quadrature.

### Usage

```
quadcc(f, a, b, tol = .Machine$double.eps^0.5, ...)
```

### **Arguments**

f integrand as function, may have singularities at the endpoints.

a, b endpoints of the integration interval.

tol relative tolerence.

... Additional parameters to be passed to the function f.

### **Details**

Adaptive version of the Clenshaw-Curtis quadrature formula with an (4, 8)-point erroe term.

## Value

List with two components, value the value of the integral and the relative error error.

#### See Also

```
clenshaw_curtis
```

quadgk 271

### **Examples**

```
## Not run:
## Dilogarithm function
flog <- function(t) log(1-t)/t
quadcc(flog, 1, 0, tol = 1e-12)
# 1.644934066848128 - pi^2/6 < 1e-13
## End(Not run)</pre>
```

quadgk

Adaptive Gauss-Kronrod Quadrature

### **Description**

Adaptive Gauss-Kronrod Quadrature.

## Usage

```
quadgk(f, a, b, tol = .Machine$double.eps^0.5, ...)
```

## **Arguments**

f integrand as function, may have singularities at the endpoints.

a, b endpoints of the integration interval.

tol relative tolerence.

... Additional parameters to be passed to the function f.

#### **Details**

Adaptive version of the (7, 15)-point Gauss-Kronrod quadrature formula, where in each recursion the error is taken as the difference between these two estimated integrals.

#### Value

Value of the integration. The relative error should be of the same order of magnitude as the relative tolerance (or much smaller).

#### Note

Uses the same nodes and weights as the quadQK15 procedure in the QUADPACK library.

### See Also

```
gauss_kronrod
```

272 quadgr

### **Examples**

```
## Dilogarithm function
flog <- function(t) log(1-t)/t
quadgk(flog, 1, 0, tol = 1e-12)
# 1.644934066848128 - pi^2/6 < 1e-13</pre>
```

quadgr

Gaussian Quadrature with Richardson Extrapolation

### **Description**

Gaussian 12-point quadrature with Richardson extrapolation.

### Usage

```
quadgr(f, a, b, tol = .Machine$double.eps^(1/2), ...)
```

### **Arguments**

f integrand as function, may have singularities at the endpoints.

a, b endpoints of the integration interval.

tol relative tolerence.

... Additional parameters to be passed to the function f.

## **Details**

quadgr uses a 12-point Gauss-Legendre quadrature. The error estimate is based on successive interval bisection. Richardson extrapolation accelerates the convergence for some integrals, especially integrals with endpoint singularities.

Through some preprocessing infinite intervals can also be handled.

#### Value

List with value and rel.err.

### Author(s)

Copyright (c) 2009 Jonas Lundgren for the Matlab function quadgr available on MatlabCentral under the BSD license.

R re-implementation by HwB, email: <a href="mailto:kwborchers@googlemail.com">hwborchers@googlemail.com</a>, in 2011.

### See Also

gaussLegendre

quadinf 273

### **Examples**

```
## Dilogarithm function
flog <- function(t) log(1-t)/t
quadgr(flog, 1, 0, tol = 1e-12)
# value
# 1.6449340668482 , is pi^2/6 = 1.64493406684823
# rel.err
# 2.07167616395054e-13</pre>
```

quadinf

Infinite Integrals

### **Description**

Iterative quadrature of functions over finite, semifinite, or infinite intervals.

### Usage

```
quadinf(f, xa, xb, tol = 1e-12, ...)
```

## Arguments

f	univariate function; needs not be vectorized.
xa	lower limit of integration; can be infinite
xb	upper limit of integration; can be infinite
tol	accuracy requested.
	additional arguments to be passed to f.

#### **Details**

quadinf implements the 'double exponential method' for fast numerical integration of smooth real functions on finite intervals. For infinite intervals, the tanh-sinh quadrature scheme is applied, that is the transformation g(t)=tanh(pi/2\*sinh(t)).

Please note that this algorithm does work very accurately for 'normal' function, but should not be applied to (heavily) oscillating functions. The maximal number of iterations is 7, so if this is returned the iteration may not have converged.

The integrand function needs *not* be vectorized.

### Value

A list with components Q the integral value, relerr the relative error, and niter the number of iterations.

#### Note

See also my remarks on R-help in September 2010 in the thread "bivariate vector numerical integration with infinite range".

274 quadl

### References

http://crd-legacy.lbl.gov/~dhbailey/dhbpapers/dhb-tanh-sinh.pdf

#### See Also

```
integrate, quadgk
```

## **Examples**

```
## We will look at the error function exp(-x^2)
f <- function(x) exp(-x^2)  # sqrt(pi)/2  theory
quadinf(f, 0, Inf)  # 0.8862269254527413
quadinf(f, -Inf, 0)  # 0.8862269254527413

f = function(x) sqrt(x) * exp(-x)  # 0.8862269254527579 exact
quadinf(f, 0, Inf)  # 0.8862269254527579

f = function(x) x * exp(-x^2)  # 1/2
quadinf(f, 0, Inf)  # 0.5

f = function(x) 1 / (1+x^2)  # 3.141592653589793 = pi
quadinf(f, -Inf, Inf)  # 3.141592653589784</pre>
```

quadl

Adaptive Lobatto Quadrature

## Description

Adaptive quadrature of functions of one variable over a finite interval.

## Usage

```
quadl(f, xa, xb, tol = .Machine$double.eps^0.5, trace = FALSE, ...)
```

## Arguments

f	a one-dimensional function; needs to be vectorized.
xa	lower limit of integration; must be finite
xb	upper limit of integration; must be finite
tol	accuracy requested.
trace	logical; shall a trace be printed?
	additional arguments to be passed to f.

### **Details**

Realizes adaptive Lobatto quadrature in R through recursive calls.

The function f needs to be vectorized though this could be changed easily.

quadv 275

### Value

A single numeric value, the computed integral.

#### Note

Compared to Gaussian quadrature, Lobatto integration include the end points of the integration interval. It is accurate for polynomials up to degree 2n-3, where n is the number of integration points.

### Author(s)

Copyright (c) 1998 Walter Gautschi for the Matlab version published as part of the referenced article. R implementation by Hans W Borchers 2011.

### References

```
Gander, W. and W. Gautschi (2000). "Adaptive Quadrature — Revisited". BIT, Vol. 40, 2000, pp. 84-101. http://www.inf.ethz.ch/personal/gander
```

### See Also

quad

### **Examples**

quadv

Vectorized Integration

### **Description**

Vectorized adaptive Simpson integration.

### Usage

```
quadv(f, a, b, tol = .Machine$double.eps^(1/2), ...)
```

276 quadv

### **Arguments**

f	univariate, vector-valued function; need not be vectorized.
a, b	endpoints of the integration interval.
tol	acuracy required for the recursion step.
	further parameters to be passed to the function f.

### **Details**

Recursive version of the adaptive Simpson quadrature, recursion is based on the maximum of all components of the function calls.

quad is not suitable for functions with singularities in the interval or at end points.

## Value

Returns a list with components Q the integral value, fcnt the number of function calls, and estim.prec the estimated precision that normally will be much too high.

### See Also

quad

```
## Examples
f1 \leftarrow function(x) c(sin(x), cos(x))
quadv(f1, 0, pi)
# $Q
# [1] 2.000000e+00 1.110223e-16
# $fcnt
# [1] 65
# $estim.prec
# [1] 4.321337e-07
f2 \leftarrow function(x) x^c(1:10)
quadv(f2, 0, 1, tol = 1e-12)
# $Q
# [1] 0.50000000 0.33333333 0.25000000 0.20000000 0.16666667
# [6] 0.14285714 0.12500000 0.111111111 0.10000000 0.09090909
# $fcnt
# [1] 505
# $estim.prec
# [1] 2.49e-10
```

quiver 277

quiver	Quiver or Velocity Plot

# Description

A quiver plot displays velocity vectors as arrows with components (u,v) at the points (x,y).

## Usage

## Arguments

x, y	x,y-coordinates of start points of the arrows.
u, v	x,y-coordinates of start points.
scale	scales the length of the arrows.
angle	angle between shaft and edge of the arrows.
length	length of the arrow edges.
• • •	more options presented to the arrows primitive.

### **Details**

The matrices x, y, u, v must all be the same size and contain corresponding position and velocity components. However, x and y can also be vectors.

### Value

Opens a graph window and plots the velocity vectors.

### See Also

```
vectorfield, arrows
```

278 rand

rand

Create Random Matrices

### **Description**

Create random matrices or random points in a unit circle (Matlab style).

### Usage

```
rand(n = 1, m = n)
randn(n = 1, m = n)
randi(imax, n = 1, m = n)
randsample(n, k, w = NULL, replacement = FALSE)
rands(n = 1, N = 1, r = 1)
randp(n = 1, r = 1)
```

### **Arguments**

n, m	integers specifying the size of the matrix
imax	integer or pair of integers
k	number of elements to return.
W	weight vector, used for discrete probabilities.
replacement	logical; sampling with or without replacement.
N	dimension of a shere, N=1 for the unit circle
r	radius of circle, default 1.

### **Details**

rand(), randn(), randi() create random matrices of size  $n \times m$ , where the default is square matrices if m is missing.

rand() uses the uniform distribution on ]0, 1[, while randn() uses the normal distribution with mean 0 and standard deviation 1.

randi() generates integers between imax[1] and imax[2] resp. 1 and imax, if imax is a scalar.

randsample() samples k elements from 1:n, with or without replacement, or returns a weighted sample (with replacement), using the weight vector w for probabilities.

rands() generates uniformly random points on an N-sphere in the N+1-dimensional space. To generate uniformly random points in the N-dim. unit cube, take points in  $S^{N-1}$  und multiply with unif(n)^(1/(N-1)).

randp() generates uniformly random points in the unit circle (or in a circle of radius r).

rand 279

### Value

Matrices of size nxm resp. a vector of length n.

```
randp() returns a pair of values representing a point in the circle, or a matrix of size (n, 2). rands() returns a matrix of size (n, N+1) with all rows being vectors of length 1.
```

#### Note

The Matlab style of setting a seed is not available; use R style set.seed(...).

### References

Knuth, D. (1981). The Art of Computer programming; Vol. 2: Seminumerical Algorithms; Chapt. 3: Random Numbers. Addison-Wesley, Reading.

### See Also

```
set.seed
```

```
rand(3)
randn(1, 5)
randi(c(1,6), 1, 10)
randsample(10, 5, replacement = TRUE, w = c(0,0,0, 1, 1, 1, 0,0,0))
P \leftarrow rands(1000, N = 1, r = 2)
U <- randp(1000, 2)
## Not run:
plot(U[, 1], U[, 2], pch = "+", asp = 1)
points(P, pch = ".")
## End(Not run)
#-- v is 2 independent normally distributed elements
# u <- randp(1); r <- t(u) %*% u
\# v \leftarrow sqrt(-2 * log(r)/r) * u
n < -5000; U < -randp(n)
R <- apply(U*U, 1, sum)</pre>
P \leftarrow sqrt(-2 * log(R)/R) * U # rnorm(2*n)
## Not run:
hist(c(P))
## End(Not run)
```

280 randcomb

randcomb

Random Combination

## Description

Generates a random combination.

## Usage

```
randcomb(a, m)
```

## Arguments

a numeric vector of some length n

m integer with  $0 \le m \le n$ 

### **Details**

Generates one random combination of the elements a of length  ${\tt m}.$ 

### Value

vector of combined elements of a

### Note

This behavior is different from Matlab/Octave, but does better correspond with the behavior of the perms() function.

### See Also

```
combs, randperm
```

```
randcomb(seq(2, 10, by=2), m = 3)
```

randperm 281

randperm

Random Permutation

## Description

Generates a random permutation.

## Usage

```
randperm(a, k)
```

### **Arguments**

a integer or numeric vector of some length n.

k integer, smaller as a or length(a).

#### **Details**

Generates one random permutation of k of the elements a, if a is a vector, or of 1:a if a is a single integer.

### Value

Vector of permuted elements of a or 1:a.

### Note

This behavior is different from Matlab/Octave, but does better correspond with the behavior of the perms() function.

### See Also

perms

```
randperm(1:6, 3)
randperm(6, 6)
randperm(11:20, 5)
randperm(seq(2, 10, by=2))
```

282 Rank

Rank

Matrix Rank

### **Description**

Provides an estimate of the rank of a matrix M.

### Usage

Rank(M)

### **Arguments**

М

Numeric matrix; vectors will be considered as column vectors.

#### **Details**

Provides an estimate of the number of linearly independent rows or columns of a matrix M. Compares an approach using QR-decomposition with one counting singular values larger than a certain tolerance (Matlab).

### Value

Matrix rank as integer between 0 and min(ncol(M), nrow(M)).

## Note

The corresponding function in Matlab is called rank, but that term has a different meaning in R.

#### References

Trefethen, L. N., and D. Bau III. (1997). Numerical Linear Algebra. SIAM, Philadelphia.

### See Also

nullspace

```
Rank(magic(10)) #=> 7
Rank(magic(100)) #=> 3 (!)
Rank(hilb(8)) #=> 8 , but qr(hilb(8))$rank says, rank is 7.
# Warning message:
# In Rank(hilb(8)) : Rank calculation may be problematic.
```

283 rat

Continuous Fractions (Matlab Style)

# Description

Generate continuous fractions for numeric values.

### Usage

```
rat(x, tol = 1e-06)
rats(x, tol = 1e-06)
```

### **Arguments**

a numeric scalar or vector.

tol tolerance; default 1e-6 to make a nicer appearance for pi.

### **Details**

rat generates continuous fractions, while rats prints the the corresponding rational representation and returns the numeric values.

### Value

rat returns a character vector of string representations of continuous fractions in the format [b0; b1, ..., b\_{n-1}]. rats prints the rational number and returns a numeric vector.

### Note

Essentially, these functions apply contfrac.

### See Also

```
numbers::contfrac
```

## **Examples**

```
rat(pi)
rats(pi)
rat(sqrt(c(2, 3, 5)), tol = 1e-15)
rats(sqrt(c(2, 3, 5)), tol = 1e-15)
```

rat

284 ratinterp

rp Rational Interpolation
---------------------------

### **Description**

Burlisch-Stoer rational interpolation.

### Usage

```
ratinterp(x, y, xs = x)
```

### **Arguments**

x	numeric vector; points on the x-axis; needs to be sorted; at least three points required.
У	numeric vector; values of the assumed underlying function; $\boldsymbol{x}$ and $\boldsymbol{y}$ must be of the same length.
xs	numeric vector; points at which to compute the interpolation; all points must lie between $min(x)$ and $max(x)$ .

### **Details**

The Burlisch-Stoer approach to rational interpolation is a recursive procedure (similar to the Newton form of polynomial interpolation) that produces a "diagonal" rational function, that is the degree of the numerator is either the same or one less than the degree of the denominator.

Polynomial interpolation will have difficulties if some kind of singularity exists in the neighborhood, even if the pole occurs in the complex plane. For instance, Runge's function has a pole at z=0.2i, quite close to the interval [-1,1].

### Value

Numeric vector representing values at points xs.

### Note

The algorithm does not yield a simple algebraic expression for the rational function found.

### References

Stoer, J., and R. Bulirsch (2002). Introduction to Numerical Analysis. Third Edition, Springer-Verlag, New York.

Fausett, L. V. (2008). Applied Numerical Analysis Using Matlab. Second Edition, Pearson Education.

#### See Also

```
rationalfit, pade
```

rationalfit 285

### **Examples**

```
## Rational interpolation of Runge's function
x <- c(-1, -0.5, 0, 0.5, 1.0)
y <- runge(x)
xs <- linspace(-1, 1)
ys <- runge(xs)
yy <- ratinterp(x, y, xs) # returns exactly the Runge function
## Not run:
plot(xs, ys, type="l", col="blue", lty = 2, lwd = 3)
points(x, y)
yy <- ratinterp(x, y, xs)
lines(xs, yy, col="red")
grid()
## End(Not run)</pre>
```

rationalfit

Rational Function Approximation

### **Description**

Fitting a rational function to data points.

### Usage

```
rationalfit(x, y, d1 = 5, d2 = 5)
```

### **Arguments**

X	numeric vector; points on the x-axis; needs to be sorted; at least three points required.
у	numeric vector; values of the assumed underlying function; x and y must be of the same length.
d1, d2	maximal degrees of numerator (d1) and denominator (d1) of the requested rational function.

#### **Details**

A rational fit is a rational function of two polynomials p1 and p2 (of user specified degrees d1 and d2) such that p1(x)/p2(x) approximates y in a least squares sense.

d1 and d2 must be large enough to get a good fit and usually d1=d2 gives good results

### Value

List with components p1 and p2 for the polynomials in numerator and denominator of the rational function.

286 rationalfit

### Note

This implementation will later be replaced by a 'barycentric rational interpolation'.

### Author(s)

Copyright (c) 2006 by Paul Godfrey for a Matlab version available from the MatlabCentral under BSD license. R re-implementation by Hans W Borchers.

#### References

Press, W. H., S. A. Teukolsky, W. T Vetterling, and B. P. Flannery (2007). Numerical Recipes: The Art of Numerical Computing. Third Edition, Cambridge University Press, New York.

#### See Also

ratinterp

```
x \leftarrow linspace(0, 15, 151); y \leftarrow sin(x)/x
rA <- rationalfit(x, y, 10, 10); p1 <- rA$p1; p2 <- rA$p2
ys <- polyval(p1,x) / polyval(p2,x)
plot(x, y, type="l", col="blue", ylim=c(-0.5, 1.0))
points(x, Re(ys), col="red") # max(abs(y-ys), na.rm=TRUE) < 1e-6
grid()
# Rational approximation of the Zeta function
x < - seq(-5, 5, by = 1/16)
y \leftarrow zeta(x)
rA <- rationalfit(x, y, 10, 10); p1 <- rA$p1; p2 <- rA$p2
ys <- polyval(p1,x) / polyval(p2,x)
plot(x, y, type="l", col="blue", ylim=c(-5, 5))
points(x, Re(ys), col="red")
grid()
# Rational approximation to the Gamma function
x \leftarrow seq(-5, 5, by = 1/32); y \leftarrow gamma(x)
rA \leftarrow rationalfit(x, y, 10, 10); p1 \leftarrow rA$p1; p2 \leftarrow rA$p2
ys <- polyval(p1,x) / polyval(p2,x)
plot(x, y, type="l", col = "blue")
points(x, Re(ys), col="red")
grid()
## End(Not run)
```

rectint 287

rectint

Rectangle Intersection Areas

### **Description**

Calculates the area of intersection of rectangles, specified by position vectors x and y.

### Usage

```
rectint(x, y)
```

## Arguments

х, у

both vectors of length 4, or both matrices with 4 columns.

### **Details**

Rectangles are specified as position vectors, that is c(x[1], x[2]) is the lower left corner, x[3] and x[4] are width and height of the rectangle. When x and y are matrices, each row is assumed to be a position vector specifying a rectangle.

### Value

Returns a scalar if x and y are vectors. If x is a n-by-4 and y a m-by-4 matrix, then it returns a n-by-m matrix R with entry (i,j) being the area rectint(x[i,j], y[j,j]).

### See Also

```
polyarea
```

```
x <- c(0.5, 0.5, 0.25, 1.00)
y <- c(0.3, 0.3, 0.35, 0.75)
rectint(x, y)
# [1] 0.0825</pre>
```

288 refindall

refi		

Find overlapping regular expression matches.

## Description

Find overlapping matches for a regular expression.

### Usage

```
refindall(s, pat, over = 1, ignorecase = FALSE)
```

### **Arguments**

s Single character string.
pat Regular expression.

over Natural number, indication how many steps to go forward after a match; defaults

to 1.

ignorecase logical, whether to ignore case.

#### **Details**

Returns the starting position of all — even overlapping — matches of the regular expression pat in the character string s.

The syntax for pattern matching has to be PERL-like.

### Value

A numeric vector with the indices of starting positions of all matches.

### Note

This effect can also be reached with the R function gregexpr(), see the example below.

#### See Also

```
regexp
```

```
refindall("ababababa", 'aba')
gregexpr('a(?=ba)', "ababababa", perl=TRUE)
refindall("AbababaBa", 'aba')
refindall("AbababaBa", 'aba', ignorecase = TRUE)
```

regexp 289

regexp	Match regular expression	
. 980%	Transit regular cupression	

## Description

Returns the positions of substrings that match the regular expression.

#### Usage

```
regexp(s, pat, ignorecase = FALSE, once = FALSE, split = FALSE)
regexpi(s, pat, once = FALSE, split = FALSE)
```

### **Arguments**

s Character string, i.e. of length 1.

pat Matching pattern as character string.

ignorecase Logical: whether case should be ignored; default: FALSE.

once Logical: whether the first are all occurrences should be found; default: all.

split Logical: should the string be splitted at the occurrences of the pattern?; default:

#### Details

no.

Returns the start and end positions and the exact value of substrings that match the regular expression. If split is choosen, the splitted strings will also be returned.

#### Value

A list with components start and end as numeric vectors indicating the start and end positions of the matches.

match contains each exact match, and split contains the character vector of splitted strings.

If no match is found all components will be NULL, except split that will contain the whole string if split = TRUE.

### Note

This is the behavior of the corresponding Matlab function, though the signature, options and return values do not match exactly. Notice the transposed parameters s and pat compared to the corresponding R function regexpr.

#### See Also

regexpr

290 regexprep

### **Examples**

```
s <- "bat cat can car COAT court cut ct CAT-scan"
pat <- 'c[aeiou]+t'
regexp(s, pat)
regexpi(s, pat)</pre>
```

regexprep

Replace string using regular expression

## **Description**

Replace string using regular expression.

## Usage

```
regexprep(s, expr, repstr, ignorecase = FALSE, once = FALSE)
```

## Arguments

s Single character string.

expr Regular expression to be matched.

repstr String that replaces the matched substring(s).

ignorecase logical, whether to ignore case.

once logical, shall only the first or all occurences be replaced.

## **Details**

Matches the regular expression against the string and replaces the first or all non-overlapping occurrences with the replacement string.

The syntax for regular expression has to be PERL-like.

#### Value

String with substrings replaced.

### Note

The Matlab/Octave variant allows a character vector. This is not possible here as it would make the return value quite complicated.

## See Also

gsub

repmat 291

## **Examples**

```
s <- "bat cat can car COAT court cut ct CAT-scan"
pat <- 'c[aeiou]+t'
regexprep(s, pat, '---')
regexprep(s, pat, '---', once = TRUE)
regexprep(s, pat, '---', ignorecase = TRUE)</pre>
```

repmat

Replicate Matrix

# Description

Replicate and tile matrix.

## Usage

```
repmat(a, n, m = n)
```

### **Arguments**

a vector or matrix to be replicated.

n, m number of times to replicate in each dimension.

### **Details**

repmat(a,m,n) creates a large matrix consisting of an m-by-n tiling of copies of a.

### Value

Returns matrix with value a replicated to the number of times in each dimension specified. Defaults to square if dimension argument resolves to a single value.

## See Also

Reshape

292 ridders

Reshape

Reshape Matrix

## Description

Reshape matrix or vector.

### Usage

```
Reshape(a, n, m)
```

## Arguments

```
a matrix or vector n, m size of the result
```

#### **Details**

Reshape(a, n, m) returns the n-by-m matrix whose elements are taken column-wise from a.

An error results if a does not have n\*m elements. If m is missing, it will be calculated from n and the size of a.

### Value

Returns matrix (or array) of the requested size containing the elements of a.

## **Examples**

```
a <- matrix(1:12, nrow=4, ncol=3)
Reshape(a, 6, 2)
Reshape(a, 6) # the same
Reshape(a, 3, 4)</pre>
```

ridders

Ridders' Method

## **Description**

Ridders' root finding method is a powerful variant of 'regula falsi' (and 'false position'). In reliability and speed, this method is competitive with Brent-Dekker and similar approaches.

## Usage

```
ridders(f, a, b, maxiter = 100, tol = .Machine$double.eps^0.5)
```

ridders 293

## **Arguments**

f function whose root is to be found.

a, b left and right interval bounds.

maxiter maximum number of iterations (function calls).

tol tolerance, length of the last interval.

### **Details**

Given a bracketing interval  $[x_1, x_2]$ , the method first calculates the midpoint  $x_3 = (x_1 + x_2)/2$  and the uses an updating formula

$$x_4 = x_3 + (x_3 - x_1) \frac{sgn(f(x_1) - f(x_2))f(x_3)}{\sqrt{f(x_3)^2 - f(x_1)f(x_2)}}$$

#### Value

Returns a list with components

root root of the function.

f. root value of the function at the found root.

niter number of iterations, or more specifically: number of function calls.

estim.prec the estimated precision, coming from the last brackett.

## Note

See function f12 whose zero at  $\sqrt{e}$  is difficult to find exactly for all root finders.

### Author(s)

HwB email: <a href="mailto:</a> <a href="mailto:hwborchers@googlemail.com">hwborchers@googlemail.com</a>

## References

Press, Teukolsky, Vetterling, and Flannery (1992). Numerical Recipes in C. Cambridge University Press.

#### See Also

brent

294 rk4, rk4sys

```
f5 <- function(x) x^2 - (1 - x)^9
                                            # [-1.4, 1],
                                                            0.259 204 4937
                                            # [-0.8, 1.6], 0.536 741 6626
f6 <- function(x) (x-1)*exp(-9*x) + x^9
f7 <- function(x) x^2 + \sin(x/9) - 1/4
                                            # [-0.5, 1.9], 0.4475417621
f8 <- function(x) 1/8 * (9 - 1/x)
                                          # [0.001, 1.201], 0.111 111 1111
f9 <- function(x) tan(x) - x - 0.0463025 \# [-0.9, 1.5], 0.500 000 0340
f10 <- function(x)</pre>
                                            # [0.4, 1],
                                                            0.679 808 9215
            x^2 + x*\sin(sqrt(75)*x) - 0.2
f11 <- function(x) x^9 + 0.0001
                                            # [-1.2, 0], -0.359 381 3664
f12 <- function(x)</pre>
                                            # [1, 3.4],
                                                           1.648 721 27070
            log(x) + x^2/(2*exp(1)) - 2 * x/sqrt(exp(1)) + 1
r <- ridders(f1 , 0, 1.2);
                                 r$root; r$niter # 18
r < - ridders(f2, 0.4, 1.6);
                                 r$root; r$niter # 14
r <- ridders(f3 ,-0.5, 1.9);
                                 r$root; r$niter # 20
r <- ridders(f4 ,-0.5, 0.7);
                                 r$root; r$niter # 12
r <- ridders(f5 ,-1.4, 1);
                                 r$root; r$niter # 16
r <- ridders(f6 ,-0.8, 1.6);
                                 r$root; r$niter # 20
r \leftarrow ridders(f7, -0.5, 1.9);
                                 r$root; r$niter # 16
r <- ridders(f8 ,0.001, 1.201); r$root; r$niter # 18
r <- ridders(f9 ,-0.9, 1.5);
                                 r$root; r$niter # 20
r <- ridders(f10,0.4, 1);
                                 r$root; r$niter # 14
r <- ridders(f11,-1.2, 0);
                                 r$root; r$niter # 12
r <- ridders(f12,1, 3.4);
                                 r$root; r$niter # 30, err = 1e-5
## Not run:
## Use ridders() with Rmpfr
options(digits=16)
library("Rmpfr") # unirootR
prec <- 256
.N <- function(.) mpfr(., precBits = prec)</pre>
f12 <- function(x) {
    e1 <- exp(.N(1))
    log(x) + x^2/(2*e1) - 2*x/sqrt(e1) + 1
sqrte <- sqrt(exp(.N(1))) # 1.648721270700128...</pre>
                           # 0
f12(sqrte)
unirootR(f12, interval=mpfr(c(1, 3.4), prec), tol=1e-20)
# $root
# 1 'mpfr' number of precision 200 bits
# [1] 1.648721270700128...
ridders(f12, .N(1), .N(3.4), maxiter=200, tol=1e-20)
# $root
# 1 'mpfr' number of precision 200
                                      bits
# [1] 1.648721270700128...
## End(Not run)
```

rk4, rk4sys 295

## **Description**

Classical Runge-Kutta of order 4.

### Usage

```
rk4(f, a, b, y0, n)
rk4sys(f, a, b, y0, n)
```

## **Arguments**

```
f function in the differential equation y'=f(x,y); defined as a function R\times R^m\to R^m, where m is the number of equations. a, b endpoints of the interval.  
y0 starting values; for m equations y0 needs to be a vector of length m.  
n the number of steps from a to b.
```

#### **Details**

Classical Runge-Kutta of order 4 for (systems of) ordinary differential equations with fixed step size.

#### Value

List with components x for grid points between a and b and y an n-by-m matrix with solutions for variables in columns, i.e. each row contains one time stamp.

#### Note

This function serves demonstration purposes only.

### References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

#### See Also

```
ode23, deval
```

296 rkf54

```
sol <- rk4(f, 0, 2, 0, 50)
## Not run:
x \leftarrow seq(0, 2, length.out = 51)
plot(x, x*exp(-x^2), type = "l", col = "red")
points(sol$x, sol$y, pch = "*")
grid()
## End(Not run)
## Example2: Chemical process
  f <- function(t, u) {</pre>
    u1 \leftarrow u[3] - 0.1 * (t+1) * u[1]
    u2 \leftarrow 0.1 * (t+1) * u[1] - 2 * u[2]
    u3 \leftarrow 2 * u[2] - u[3]
    return(c(u1, u2, u3))
  }
u0 <- c(0.8696, 0.0435, 0.0870)
a <- 0; b <- 40
n <- 40
sol <- rk4sys(f, a, b, u0, n)</pre>
## Not run:
matplot(sol$x, sol$y, type = "l", lty = 1, lwd = c(2, 1, 1),
        col = c("darkred", "darkblue", "darkgreen"),
        xlab = "Time [min]", ylab= "Concentration [Prozent]",
        main = "Chemical composition")
grid()
## End(Not run)
```

rkf54

Runge-Kutta-Fehlberg

## **Description**

Runge-Kutta-Fehlberg with adaptive step size.

### Usage

## **Arguments**

f	function in the differential equation $y' = f(x, y)$ .
a, b	endpoints of the interval.
y0	starting values at a.
tol	relative tolerance, used for determining the step size.
control	list for influencing the step size with components hmin, hmax, the minimal, maximal step size jmax, the maximally allowed number of steps.
	additional parameters to be passed to the function.

rkf54 297

#### **Details**

Runge-Kutta-Fehlberg is a kind of Runge-Kutta method of solving ordinary differential equations of order (5, 4) with variable step size.

"At each step, two different approximations for the solution are made and compared. If the two answers are in close agreement, the approximation is accepted. If the two answers do not agree to a specified accuracy, the step size is reduced. If the answers agree to more significant digits than required, the step size is increased."

Some textbooks promote the idea to use the five-order formula as the accepted value instead of using it for error estimation. This approach is taken here, that is why the function is called rkf54. The idea is still debated as the accuracy determinations appears to be diminished.

#### Value

List with components x for grid points between a and b and y the function values of the numerical solution.

### Note

This function serves demonstration purposes only.

#### References

Stoer, J., and R. Bulirsch (2002). Introduction to Numerical Analysis. Third Edition, Springer-Verlag, New York.

Mathematica code associated with the book:

Mathews, J. H., and K. D. Fink (2004). Numerical Methods Using Matlab. Fourth Edition, Prentice Hall.

http://math.fullerton.edu/mathews/software/software.htm.

#### See Also

```
rk4, ode23
```

298 rmserr

```
lines(sol12$x, sol12$y)
points(sol21$x, sol21$y, pch = "*", col = "blue")
lines(sol22$x, sol22$y)
grid()
## End(Not run)
```

rmserr

Accuracy Measures

## Description

Calculates different accuracy measures, most prominently RMSE.

## Usage

```
rmserr(x, y, summary = FALSE)
```

### **Arguments**

x, y two vectors of real numbers

summary logical; should a summary be printed to the screen?

## **Details**

Calculates six different measures of accuracy for two given vectors or sequences of real numbers:

MAE	Mean Absolute Error
MSE	Mean Squared Error
<b>RMSE</b>	Root Mean Squared Error
MAPE	Mean Absolute Percentage Error
<b>LMSE</b>	Normalized Mean Squared Error
rSTD	relative Standard Deviation

## Value

Returns a list with different accuracy measures.

#### Note

Often used in Data Mining for predicting the accuracy of predictions.

#### References

Gentle, J. E. (2009). Computational Statistics, section 10.3. Springer Science+Business Media LCC, New York.

romberg 299

## **Examples**

```
x <- rep(1, 10)
y <- rnorm(10, 1, 0.1)
rmserr(x, y, summary = TRUE)</pre>
```

romberg

Romberg Integration

## Description

Romberg Integration

## Usage

```
romberg(f, a, b, maxit = 25, tol = 1e-12, ...)
```

## Arguments

f	function to be integrated.
a, b	end points of the interval.
maxit	maximum number of iterations.
tol	requested tolerance.
	variables to be passed to the function.

#### **Details**

Simple Romberg integration with an explicit Richardson method applied to a series of trapezoidal integrals. This scheme works best with smooth and non-oscillatory functions and needs the least number of function calls among all integration routines.

The function does *not* need to be vectorized.

## Value

List of value, number or iterations, and relative error.

### Note

Using a trapezoid formula Romberg integration will use 2\*(2^iter-1)+iter function calls. By remembering function values this could be reduced to 2^iter+1 calls.

### References

Chapra, S. C., and R. P. Canale (2006). Numerical Methods for Engineers. Fifth Edition, McGraw-Hill, New York.

300 roots

## See Also

```
integrate, quadgr
```

## **Examples**

roots

Polynomial Roots

## **Description**

Computes the roots of the polynomial p.

## Usage

roots(p)

#### **Arguments**

р

vector of real numbers representing the polynomial

#### **Details**

For solution the function computes the eigenvalues of the companion matrix.

At the moment, only real coefficients are allowed.

## Value

a vector holding the roots of the polynomial

### See Also

```
polyroot
```

```
roots(c(1, 0, 1, 0, 0)) # 0 0 1i -1i
p <- Poly(c(-2, -1, 0, 1, 2))
roots(p)
```

rortho 301

rortho

Generate Random Orthogogonal Matrix

## **Description**

Generates random orthogonal matrix of size n.

Will be needed in applications that explore high-dimensional data spaces, for example optimization procedures or Monte Carlo methods.

## Usage

```
rortho(n)
```

## **Arguments**

n

positive integer.

### **Details**

Uses the idea of the Stewart 1980, "The Efficient Generation of Random Orthogonal Matrices with an Application to Condition Estimators", to apply the Householder transformation to a uniformly distributed random vector.

#### Value

Orthogonal matrix Q of size n, that is Q \*\* t(Q) is the unit matrix of size n.

## **Examples**

```
Q \leftarrow rortho(5)
zapsmall(Q \% \% t(Q))
zapsmall(t(Q) \% \% Q)
```

rosser

Rosser Matrix

## Description

Generate the Rosser matrix.

## Usage

```
rosser()
```

302 rot90

### **Details**

This is a classic symmetric eigenvalue test problem. It has a double eigenvalue, three nearly equal eigenvalues, dominant eigenvalues of opposite sign, a zero eigenvalue, and a small, nonzero eigenvalue.

### Value

```
matrix of size 8 x 8
```

### See Also

wilkinson

## **Examples**

```
rosser()
```

rot90

Matrix Rotation

## **Description**

Rotate matrices for 90, 180, or 270 degrees..

## Usage

```
rot90(a, k = 1)
```

### **Arguments**

a numeric or complex matrix

k scalar integer number of times the matrix will be rotated for 90 degrees; may be negative.

### **Details**

Rotates a numeric or complex matrix for 90 (k = 1), 180 (k = 2) or 270 (k = 3 or k = -1) degrees. Value of k is taken mod 4.

### Value

the original matrix rotated

```
a <- matrix(1:12, nrow=3, ncol=4, byrow=TRUE)
rot90(a)
rot90(a, 2)
rot90(a, -1)</pre>
```

rref 303

rref

Reduced Row Echelon Form

## **Description**

Produces the reduced row echelon form of A using Gauss Jordan elimination with partial pivoting.

## Usage

rref(A)

## **Arguments**

Α

numeric matrix.

### **Details**

A matrix of "row-reduced echelon form" has the following characteristics:

- 1. All zero rows are at the bottom of the matrix
- 2. The leading entry of each nonzero row after the first occurs to the right of the leading entry of the previous row.
- 3. The leading entry in any nonzero row is 1.
- 4. All entries in the column above and below a leading 1 are zero.

Roundoff errors may cause this algorithm to compute a different value for the rank than rank, orth or null.

## Value

A matrix the same size as m.

### Note

This serves demonstration purposes only; don't use for large matrices.

## References

Weisstein, Eric W. "Echelon Form." From MathWorld – A Wolfram Web Resource. http://mathworld.wolfram.com/EchelonForm.html

## See Also

qr.solve

304 runge

### **Examples**

```
A \leftarrow matrix(c(1, 2, 3, 1, 3, 2, 3, 2, 1), 3, 3, byrow = TRUE)
rref(A)
       [,1] [,2] [,3]
# [1,]
               0
          1
# [2,]
                     0
          0
               1
# [3,]
          0
                    1
A <- matrix(data=c(1, 2, 3, 2, 5, 9, 5, 7, 8,20, 100, 200),
            nrow=3, ncol=4, byrow=FALSE)
rref(A)
         0
              0 120
   1
    0
         1
              0
                   0
    0
         0
              1 -20
# Use rref on a rank-deficient magic square:
A = magic(4)
R = rref(A)
zapsmall(R)
                   1
    1
         0
              0
    0
                   3
         1
              0
                  -3
    0
         0
              1
                   0
         0
```

runge

Runge Function

## **Description**

Runge's test function for interpolation techniques.

## Usage

```
runge(x)
```

## **Arguments**

Χ

numeric scalar.

### **Details**

Runge's function is a classical test function for interpolation and and approximation techniques, especially for equidistant nodes.

For example, when approximating the Runge function on the interval [-1, 1], the error at the endpoints will diverge when the number of nodes is increasing.

## Value

Numerical value of the function.

runs.test 305

### See Also

fnorm

### **Examples**

```
## Not run:
x <- seq(-1, 1, length.out = 101)
y <- runge(x)
plot(x, y, type = "l", lwd = 2, col = "navy", ylim = c(-0.2, 1.2))
grid()

n <- c(6, 11, 16)
for (i in seq(along=n)) {
    xp <- seq(-1, 1, length.out = n[i])
    yp <- runge(xp)
    p <- polyfit(xp, yp, n[i]-1)
    y <- polyval(p, x)
    lines(x, y, lty=i) }

## End(Not run)</pre>
```

runs.test

The Runs Test, or Wald-Wolfowitz Test

### **Description**

The "Runs Test", or Wald-Wolfowitz Test for Randomness

### Usage

```
runs.test(x)
```

#### **Arguments**

Χ

vector with only two different values.

#### Details

The Runs Test is a non-parametric test for checking the randomness of a dichotomous sequence, i.e. with only two different values. The test counts the number of 'runs', subsequences consisting of the same adjacent element.

The two characteristic elements of the sequence need not have the same probability. The null hypothesis is the assumption that the elements are independently drawn from from the conditional distribution given by the frequncy distribution within the sequence.

### Value

Returns a list with components \$Z the test statistics, and \$p.value the p-value for the null hypothesis.

306 savgol

### References

The 'dieharder' website at http://www.phy.duke.edu/~rgb/General/dieharder.php

#### See Also

```
chisq.test, RDieHarder::dieharder
```

### **Examples**

```
runs.test(x1)
## $Z
## [1] -0.1617764
## $p.value
## [1] 0.8714819
x2 <- rep(c(0, 1), 50)
runs.test(x2)
## $Z
## [1] 9.849873
## $p.value
## [1] 0
# Which sequence is random?
0,0,1,0,0,1,0,0,0,1,0,1,0,1,1,0,1,0,0,1,1,1,0,1)
1,0,1,0,1,1,1,0,0,0,0,0,1,0,1,0,1,1,0,0,1,1,1,0)
runs.test(x3) # null hypotheses rejected at 0.05 level
## $Z
## [1] 2.05555
## $p.value
## [1] 0.03982587
runs.test(x4) # randomness is very probable
## $Z
## [1] 0.002947558
## $p.value
## [1] 0.9976482
```

savgol

Savitzky-Golay Smoothing

## Description

Polynomial filtering method of Savitzky and Golay.

savgol 307

### Usage

```
savgol(T, fl, forder = 4, dorder = 0)
```

### **Arguments**

T Vector of signals to be filtered.

f1 Filter length (for instance fl = 51..151), has to be odd.

forder Filter order (2 = quadratic filter, 4 = quartic).

dorder Derivative order (0 = smoothing, 1 = first derivative, etc.).

### **Details**

Savitzky-Golay smoothing performs a local polynomial regression on a series of values which are treated as being equally spaced to determine the smoothed value for each point. Methods are also provided for calculating derivatives.

#### Value

Vector representing the smoothed time series.

#### Note

For derivatives T2 has to be divided by the step size to the order (and to be multiplied by k! — the sign appears to be wrong).

## Author(s)

Peter Riegler implemented a Matlab version in 2001. Based on this, Hans W. Borchers published an R version in 2003.

#### References

See Numerical Recipes, 1992, Chapter 14.8, for details.

## See Also

```
RTisean::sav_gol, signal::sgolayfilt, whittaker.
```

```
## Not run:
# *** Sinosoid test function ***
ts <- sin(2*pi*(1:1000)/200)
t1 <- ts + rnorm(1000)/10
t2 <- savgol(t1, 51)
plot( 1:1000, t1, col = "grey")
lines(1:1000, ts, col = "blue")
lines(1:1000, t2, col = "red")
# t3 <- whittaker(t1, lambda = 1600)
# lines(1:1000, t3, col = "darkgreen", lwd = 2)</pre>
```

308 segm\_distance

```
Whittacker Smoothing
   Paul Eilers, 2002 (Matlab) and Nicholas Lewin-Koh, 2004 (R/S) \,
whittaker <- function(y, lambda, d = 2){</pre>
   Smoothing with a finite difference penalty
            signal to be smoothed
   lambda: smoothing parameter (rough 50..1e4 smooth)
   d: order of differences in penalty (generally 2)
   require(SparseM, warn.conflicts = FALSE)
   m <- length(y)</pre>
   E <- as(m, "matrix.diag.csr")</pre>
    class(E) <- "matrix.csr"</pre>
    Dmat <- diff(E, differences = d)</pre>
   B <- E + (lambda * t(Dmat) %*% Dmat)
    z \leftarrow solve(B, y)
    return(z)
}
## End(Not run)
```

segm\_distance

Segment Distance

## **Description**

The minimum distance between a point and a segment, or the minimum distance between points of two segments.

### Usage

```
segm_distance(p1, p2, p3, p4 = c())
```

## **Arguments**

p1, p2 end points of the first segment.

p3, p4 end points of the second segment, or the point p3 alone if p4 is NULL.

## **Details**

If p4=c(), determines the orthogonal line to the segment through the single point and computes the distance to the intersection point.

Otherwise, it computes the distances of all four end points to the other segment and takes the minimum of those.

segm\_intersect 309

### Value

Returns a list with component 1 the minimum distance and components p, q the two nearest points. If p4=c() then point p lies on the segment and q is p4.

#### Note

The interfaces of segm\_intersect and segm\_distance should be brought into line.

## See Also

```
segm_intersect
```

## **Examples**

segm\_intersect

Segment Intersection

## Description

Do two segments have at least one point in common?

# Usage

```
segm_intersect(s1, s2)
```

## **Arguments**

s1, s2 Two segments, represented by their end points; i.e., s <- rbind(p1, p2) when p1, p2 are the end points.

310 segm\_intersect

### **Details**

First compares the 'bounding boxes', and if those intersect looks at whether the other end points lie on different sides of each segment.

#### Value

Logical, TRUE if these segments intersect.

#### Note

Should be written without reference to the cross function. Should also return the intersection point, see the example.

#### References

Cormen, Th. H., Ch. E. Leiserson, and R. L. Rivest (2009). Introduction to Algorithms. Third Edition, The MIT Press, Cambridge, MA.

#### See Also

```
segm_distance
```

```
## Not run:
plot(c(0, 1), c(0, 1), type="n",
     xlab = "", ylab = "", main = "Segment Intersection")
grid()
for (i in 1:20) {
s1 <- matrix(runif(4), 2, 2)</pre>
s2 <- matrix(runif(4), 2, 2)</pre>
if (segm_intersect(s1, s2)) {
    clr <- "red"
    p1 <- s1[1, ]; p2 <- s1[2, ]; p3 <- s2[1, ]; p4 <- s2[2, ]
    A \leftarrow cbind(p2 - p1, p4 - p3)
    b \leftarrow (p3 - p1)
    a <- solve(A, b)
    points((p1 + a[1]*(p2-p1))[1], (p1 + a[1]*(p2-p1))[2], pch = 19, col = "blue")
} else
    clr <- "darkred"
lines(s1[,1], s1[, 2], col = clr)
lines(s2[,1], s2[, 2], col = clr)
## End(Not run)
```

semilogx,semilogy 311

semilogx,semilogy

Semi-logarithmic Plots (Matlab Style)

## Description

Generates semi- and double-logarithmic plots.

# Usage

```
semilogx(x, y, ...)
semilogy(x, y, ...)
loglog(x, y, ...)
```

## Arguments

```
x, yx-, y-coordinates.additional graphical parameters passed to the plot function.
```

### **Details**

Plots data in logarithmic scales for the x-axis or y-axis, or uses logarithmic scales in both axes, and adds grid lines.

## Value

Generates a plot, returns nothing.

#### Note

Matlab's logarithmic plots find a more appropriate grid.

## See Also

```
plot with log= option.
```

```
## Not run:
x <- logspace(-1, 2)
loglog(x, exp(x), type = 'b')
## End(Not run)</pre>
```

312 sigmoid

sigmoid

Sigmoid Function

#### **Description**

Sigmoid function (aka sigmoidal curve or logistic function).

## Usage

```
sigmoid(x, a = 1, b = 0)
logit(x, a = 1, b = 0)
```

## Arguments

x numeric vector.

a, b parameters.

#### **Details**

The sigmoidal function with parameters a, b is the function

$$y = 1/(1 + e^{-a(x-b)})$$

The sigmoid function is also the solution of the ordinary differential equation

$$y' = y(1 - y)$$

with y(0) = 1/2 and has an indefinite integral  $\ln(1 + e^x)$ .

The logit function is the inverse of the sigmoid function and is (therefore) omly defined between 0 and 1. Its definition is

$$y = b + 1/alog(x/(1-x))$$

#### Value

Numeric/complex scalar or vector.

simpadpt 313

S1	am	ad	pt

Adaptive Simpson Quadrature

## Description

Numerically evaluate an integral using adaptive Simpson's rule.

### Usage

```
simpadpt(f, a, b, tol = 1e-6, ...)
```

## **Arguments**

f univariate function, the integrand.	f	univariate	function,	the integrand.
---------------------------------------	---	------------	-----------	----------------

a, b lower limits of integration; must be finite.

tol relative tolerance

... additional arguments to be passed to f.

## **Details**

Approximates the integral of the function f from a to b to within an error of tol using recursive adaptive Simpson quadrature.

## Value

A numerical value or vector, the computed integral.

## Note

Based on code from the book by Quarteroni et al., with some tricks borrowed from Matlab and Octave.

### References

Quarteroni, A., R. Sacco, and F. Saleri (2007). Numerical Mathematics. Second Edition, Springer-Verlag, Berlin Heidelberg.

### See Also

```
quad, simpson2d
```

314 simpson2d

### **Examples**

```
myf \leftarrow function(x, n) 1/(x+n) \# 0.0953101798043249 , log((n+1)/n) for n=10
simpadpt(myf, 0, 1, n = 10) # 0.095310179804535
## Dilogarithm function
flog <- function(t) log(1-t) / t # singularity at t=1, almost at t=0
dilog <- function(x) simpadpt(flog, x, 0, tol = 1e-12)
dilog(1) # 1.64493406685615
          # 1.64493406684823 = pi^2/6
## Not run:
N <- 51
xs \leftarrow seq(-5, 1, length.out = N)
ys <- numeric(N)</pre>
for (i in 1:N) ys[i] <- dilog(xs[i])</pre>
plot(xs, ys, type = "l", col = "blue",
             main = "Dilogarithm function")
grid()
## End(Not run)
```

simpson2d

Double Simpson Integration

### **Description**

Numerically evaluate double integral by 2-dimensional Simpson method.

## Usage

```
simpson2d(f, xa, xb, ya, yb, nx = 128, ny = 128, ...)
```

## Arguments

f	function of two variables, the integrand.
xa, xb	left and right endpoint for first variable.
ya, yb	left and right endpoint for second variable.
nx, ny	number of intervals in x- and y-direction.
	additional parameters to be passed to the integrand.

## **Details**

The 2D Simpson integrator has weights that are most easily determined by taking the outer product of the vector of weights for the 1D Simpson rule.

### Value

Numerical scalar, the value of the integral.

size 315

## Note

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#### See Also

```
dblquad, quad2d
```

## **Examples**

```
f1 <- function(x, y) x^2 + y^2

simpson2d(f1, -1, 1, -1, 1) # 2.666666667 , i.e. 8/3 . err = 0

f2 <- function(x, y) y*sin(x)+x*cos(y)

simpson2d(f2, pi, 2*pi, 0, pi) # -9.869604401 , i.e. -pi^2, err = 2e-8

f3 <- function(x, y) sqrt((1 - (x^2 + y^2)) * (x^2 + y^2 <= 1))

simpson2d(f3, -1, 1, -1, 1) # 2.094393912 , i.e. 2/3*pi , err = 1e-6
```

size

Size of Matrix

## Description

Provides the dimensions of x.

## Usage

```
size(x, k)
```

## Arguments

```
x vector, matrix, or arrayk integer specifying a particular dimension
```

## **Details**

Returns the number of dimensions as length(x).

Vector will be treated as a single row matrix.

## Value

vector containing the dimensions of x, or the k-th dimension if k is not missing.

## Note

The result will differ from Matlab when x is a character vector.

316 softline

### See Also

dim

#### **Examples**

```
size(1:8)
size(matrix(1:8, 2, 4)) # 2 4
size(matrix(1:8, 2, 4), 2) # 4
size(matrix(1:8, 2, 4), 3) # 1
```

softline

Soft (Inexact) Line Search

## Description

Fletcher's inexact line search algorithm.

## Usage

```
softline(x0, d0, f, g = NULL)
```

## Arguments

x0	initial point for linesearch.
d0	search direction from x0.
f	real function of several variables that is to be minimized.
g	gradient of objective function f; computed numerically if not provided.

#### **Details**

Many optimization methods have been found to be quite tolerant to line search imprecision, therefore inexact line searches are often used in these methods.

### Value

Returns the suggested inexact optimization paramater as a real number a0 such that x0+a0\*d0 should be a reasonable approximation.

## Note

Matlab version of an inexact linesearch algorithm by A. Antoniou and W.-S. Lu in their textbook "Practical Optimization". Translated to R by Hans W Borchers.

#### References

Fletcher, R. (1980). Practical Methods of Optimization, Volume 1., Section 2.6. Wiley, New York. Antoniou, A., and W.-S. Lu (2007). Practical Optimization: Algorithms and Engineering Applications. Springer Science+Business Media, New York.

sorting 317

## See Also

gaussNewton

### **Examples**

```
## Himmelblau function
f_himm <- function(x) (x[1]^2 + x[2] - 11)^2 + (x[1] + x[2]^2 - 7)^2
g_himm <- function(x) {
    w1 <- (x[1]^2 + x[2] - 11); w2 <- (x[1] + x[2]^2 - 7)
    g1 <- 4*w1*x[1] + 2*w2; g2 <- 2*w1 + 4*w2*x[2]
    c(g1, g2)
}
# Find inexact minimum from [6, 6] in the direction [-1, -1] !
softline(c(6, 6), c(-1, -1), f_himm, g_himm)
# [1] 3.458463
# Find the same minimum by using the numerical gradient
softline(c(6, 6), c(-1, -1), f_himm)
# [1] 3.458463</pre>
```

sorting

Sorting Routines

### **Description**

R implementations of several sorting routines. These implementations are meant for demonstration and lecturing purposes.

## Usage

```
is.sorted(a)
testSort(n = 1000)

bubbleSort(a)
insertionSort(a)
selectionSort(a)
shellSort(a, f = 2.3)
heapSort(a)
mergeSort(a, m = 10)
mergeOrdered(a, b)
quickSort(a, m = 3)
quickSortx(a, m = 25)
```

## **Arguments**

a, b Numeric vectors to be sorted or merged.

f Retracting factor for shellSort.

318 sorting

m Size of subsets that are sorted by insertionSort when the sorting procedure is called recursively.

n Only in testSort: the length of a vector of random numbers to be sorted.

#### **Details**

bubbleSort(a) is the well-known "bubble sort" routine; it is forbiddingly slow.

insertionSort(a) sorts the array one entry at a time; it is slow, but quite efficient for small data sets.

selectionSort(a) is an in-place sorting routine that is inefficient, but noted for its simplicity.

shellSort(a, f = 2.3) exploits the fact that insertion sort works efficiently on input that is already almost sorted. It reduces the gaps by the factor f; f=2.3 is said to be a reasonable choice.

heapSort(a) is not yet implemented.

mergeSort(a, m = 10) works recursively, merging already sorted parts with mergeOrdered. m should be between3 and 1/1000 of the size of a.

mergeOrdered(a, b) works only correctly if a and a are already sorted.

quickSort(a, m = 3) realizes the celebrated "quicksort algorithm" and is the fastest of all implementations here. To avoid too deeply nested recursion with R, insertionSort is called when the size of a subset is smaller than m.

Values between 3..30 seem reasonable and smaller values are better, with the risk of running into a too deeply nested recursion.

quickSort(a, m = 25) is an extended version where the split is calculated more carefully, but in general this approach takes too much time.

Values for m are 20..40 with m=25 favoured.

testSort(n = 1000) is a test routine, e.g. for testing your computer power. On an iMac, quickSort will sort an array of size 1,000,000 in less than 15 secs.

#### Value

All routines return the vector sorted.

is. sorted indicates logically whether the vector is sorted.

#### Note

At the moment, only increasingly sorting is possible (if needed apply rev afterwards).

#### Author(s)

HwB <hwborchers@googlemail.com>

## References

Knuth, D. E. (1973). The Art of Computer Programming, Volume 3: Sorting and Searching, Chapter 5: Sorting. Addison-Wesley Publishing Company.

sortrows 319

### See Also

sort, the internal C-based sorting routine.

## **Examples**

```
## Not run:
testSort(100)

a <- sort(runif(1000)); b <- sort(runif(1000))
system.time(y <- mergeSort(c(a, b)))
system.time(y <- mergeOrdered(a, b))
is.sorted(y)
## End(Not run)</pre>
```

sortrows

Sort Rows of a Matrix (Matlab Style)

## **Description**

Sort rows of a matrix according to values in a column.

## Usage

```
sortrows(A, k = 1)
```

## **Arguments**

A numeric matrix.

k number of column to sort the matrix accordingly.

### **Details**

sortrows(A, k) sorts the rows of the matrix A such that column k is increasingly sorted.

### Value

Returns the sorted matrix.

### See Also

sort

```
A <- magic(5)
sortrows(A)
sortrows(A, k = 2)
```

320 spinterp

spinterp

Monotone (Shape-Preserving) Interpolation

## Description

Monotone interpolation preserves the monotonicity of the data being interpolated, and when the data points are also monotonic, the slopes of the interpolant should also be monotonic.

#### Usage

```
spinterp(x, y, xp)
```

## **Arguments**

x, y x- and y-coordinates of the points that shall be interpolated.

xp points that should be interpolated.

### **Details**

This implementation follows a cubic version of the method of Delbourgo and Gregory. It yields 'shaplier' curves than the Stineman method.

The calculation of the slopes is according to recommended practice:

- monotonic and convex -> harmonic
- monotonic and nonconvex -> geometric
- nonmonotonic and convex -> arithmetic
- nonmonotonic and nonconvex -> circles (Stineman) [not implemented]

The choice of supplementary coefficients r[i] depends on whether the data are montonic or convex or both:

- monotonic, but not convex
- otherwise

and that can be detected from the data. The choice r[i]=3 for all i results in the standard cubic Hermitean rational interpolation.

### Value

The interpolated values at all the points of xp.

#### Note

At the moment, the data need to be monotonic and the case of convexity is not considered.

## References

Stan Wagon (2010). Mathematica in Action. Third Edition, Springer-Verlag.

spinterp 321

### See Also

```
stinepack::stinterp, demography::cm.interp
```

```
data1 <- list(x = c(1,2,3,5,6,8,9,11,12,14,15),
              y = c(rep(10,6), 10.5, 15, 50, 60, 95))
data2 <- list(x = c(0,1,4,6.5,9,10),
              y = c(10,4,2,1,3,10)
data3 <- list(x = c(7.99, 8.09, 8.19, 8.7, 9.2, 10, 12, 15, 20),
              y = c(0, 0.000027629, 0.00437498, 0.169183, 0.469428,
                     0.94374, 0.998636, 0.999919, 0.999994))
data4 \leftarrow list(x = c(22, 22.5, 22.6, 22.7, 22.8, 22.9,
                     23,23.1,23.2,23.3,23.4,23.5,24),
              y = c(523, 543, 550, 557, 565, 575,
                     590,620,860,915,944,958,986))
data5 <- list(x = c(0,1.1,1.31,2.5,3.9,4.4,5.5,6,8,10.1),
               y = c(10.1, 8, 4.7, 4.0, 3.48, 3.3, 5.8, 7, 7.7, 8.6))
data6 <- list(x = c(-0.8, -0.75, -0.3, 0.2, 0.5),
              y = c(-0.9, 0.3, 0.4, 0.5, 0.6))
data7 <- list(x = c(-1, -0.96, -0.88, -0.62, 0.13, 1),
              y = c(-1, -0.4, 0.3, 0.78, 0.91, 1))
data8 <- list(x = c(-1, -2/3, -1/3, 0.0, 1/3, 2/3, 1),
              y = c(-1, -(2/3)^3, -(1/3)^3, -(1/3)^3, (1/3)^3, (1/3)^3, (1/3)^3)
## Not run:
opr <- par(mfrow=c(2,2))
# These are well-known test cases:
D <- data1
plot(D, ylim=c(0, 100)); grid()
xp \leftarrow seg(1, 15, len=51); yp \leftarrow spinterp(D$x, D$y, xp)
lines(spline(D), col="blue")
lines(xp, yp, col="red")
D <- data3
plot(D, ylim=c(0, 1.2)); grid()
xp \leftarrow seg(8, 20, len=51); yp \leftarrow spinterp(D$x, D$y, xp)
lines(spline(D), col="blue")
lines(xp, yp, col="red")
D <- data4
plot(D); grid()
xp <- seq(22, 24, len=51); yp <- spinterp(D$x, D$y, xp)
lines(spline(D), col="blue")
lines(xp, yp, col="red")
# Fix a horizontal slope at the end points
D <- data8
x \leftarrow c(-1.05, D$x, 1.05); y \leftarrow c(-1, D$y, 1)
```

322 sqrtm,rootm

```
plot(D); grid()
xp <- seq(-1, 1, len=101); yp <- spinterp(x, y, xp)
lines(spline(D, n=101), col="blue")
lines(xp, yp, col="red")
par(opr)
## End(Not run)</pre>
```

sgrtm, rootm

Matrix Square and p-th Roots

## **Description**

Computes the matrix square root and matrix p-th root of a nonsingular real matrix.

## Usage

```
sqrtm(A, kmax = 20, tol = .Machine$double.eps^(1/2))
signm(A, kmax = 20, tol = .Machine$double.eps^(1/2))
rootm(A, p, kmax = 20, tol = .Machine$double.eps^(1/2))
```

#### Arguments

A numeric, i.e. real, matrix.
p p-th root to be taken.

kmax maximum number of iterations.

tol absolut tolerance, norm distance of A and B^p.

#### Details

A real matrix may or may not have a real square root; if it has no real negative eigenvalues. The number of square roots can vary from two to infinity. A positive definite matric has one distinguished square root, called the principal one, with the property that the eigenvalues lie in the segment  $\{z \mid -pi/p < arg(z) < pi/p\}$  (for the p-th root).

The matrix square root sqrtm(A) is computed here through the Denman-Beavers iteration (see the references) with quadratic rate of convergence, a refinement of the common Newton iteration determining roots of a quadratic equation.

The matrix p-th root rootm(A) is computed as a complex integral

$$A^{1/p} = \frac{p\sin(\pi/p)}{\pi} A \int_0^\infty (x^p I + A)^{-1} dx$$

applying the trapezoidal rule along the unit circle.

One application is the computation of the matrix logarithm as

$$\log A = 2^k \log A^{1/2^k}$$

sqrtm,rootm 323

such that the argument to the logarithm is close to the identity matrix and the Pade approximation can be applied to  $\log(I + X)$ .

The matrix sector function is defined as  $sectm(A,m)=(A^m)^{-1/p}%*%A$ ; for p=2 this is the matrix sign function.

```
S=signm(A) is real if A is and has the following properties:
```

```
S^2=Id; SA=AS
```

```
singm([0 A; B 0])=[0 C; C^{-1} 0] where C=A(BA)^{-1}
```

These functions arise in control theory.

#### Value

sqrtm(A) returns a list with components

B square root matrix of A.

Binv inverse of the square root matrix.

k number of iterations.

acc accuracy or absolute error.

rootm(A) returns a list with components

B square root matrix of A. k number of iterations.

acc accuracy or absolute error.

If k is negative the iteration has not converged.

signm just returns one matrix, even when there was no convergence.

#### Note

The p-th root of a positive definite matrix can also be computed from its eigenvalues as

```
E <- eigen(A)
```

V <- E\$vectors; U <- solve(V)

D <- diag(E\$values)

B <- V %\*% D^(1/p) %\*% U

or by applying the functions expm, logm in package 'expm':

```
B \leftarrow expm(1/p * logm(A))
```

As these approaches all calculate the principal branch, the results are identical (but will numerically slightly differ).

### References

N. J. Higham (1997). Stable Iterations for the Matrix Square Root. Numerical Algorithms, Vol. 15, pp. 227–242.

D. A. Bini, N. J. Higham, and B. Meini (2005). Algorithms for the matrix pth root. Numerical Algorithms, Vol. 39, pp. 349–378.

324 squareform

## See Also

```
expm, expm::sqrtm
```

## **Examples**

```
A1 <- matrix(c(10, 7, 8, 7,
                7, 5, 6, 5,
                8, 6, 10, 9,
                7, 5, 9, 10), nrow = 4, ncol = 4, byrow = TRUE)
X \leftarrow sqrtm(A1)B
                  # accuracy: 2.352583e-13
A2 <- matrix(c(90.81, 8.33, 0.68, 0.06, 0.08, 0.02, 0.01, 0.01,
                0.70, 90.65, 7.79, 0.64, 0.06, 0.13, 0.02, 0.01,
                0.09, 2.27, 91.05, 5.52, 0.74, 0.26, 0.01, 0.06,
                0.02, 0.33, 5.95, 85.93, 5.30, 1.17, 1.12, 0.18,
                0.03, 0.14, 0.67, 7.73, 80.53, 8.84, 1.00, 1.06,
                0.01, 0.11, 0.24, 0.43, 6.48, 83.46, 4.07, 5.20,
                0.21, 0, 0.22, 1.30, 2.38, 11.24, 64.86, 19.79,
                0, 0, 0, 0, 0, 0, 100
              ) / 100, nrow = 8, ncol = 8, byrow = TRUE)
X < - \text{rootm}(A2, 12) \# k = 6, accuracy: 2.208596e-14
## Matrix sign function
                                         # 4x4 identity matrix
signm(A1)
B <- rbind(cbind(zeros(4,4), A1),</pre>
           cbind(eye(4), zeros(4,4)))
                                         # [0, signm(A1)$B; signm(A1)$Binv 0]
signm(B)
```

squareform

Format Distance Matrix (Matlab Style)

## **Description**

Format or generate a distance matrix.

## Usage

```
squareform(x)
```

### **Arguments**

x numeric vector or matrix.

std 325

# **Details**

If x is a vector as created by the dist function, it converts it into a fulll square, symmetric matrix. And if x is a distance matrix, i.e. square, symmetric amd with zero diagonal elements, it returns the flattened lower triangular submatrix.

#### Value

Returns a matrix if x is a vector, and a vextor if x is a matrix.

# See Also

```
dist
```

# **Examples**

```
x <- 1:6
y <- squareform(x)
# 0 1 2 3
# 1 0 4 5
# 2 4 0 6
# 3 5 6 0
all(squareform(y) == x)
# TRUE</pre>
```

std

Standard Deviation (Matlab Style)

# **Description**

Standard deviation of the values of x.

# Usage

```
std(x, flag=0)
```

# **Arguments**

x numeric vector or matrix

flag numeric scalar. If 0, selects unbiased algorithm; and if 1, selects the biased version.

# **Details**

If flag = 0 the result is the square root of an unbiased estimator of the variance. std(X,1) returns the standard deviation producing the second moment of the set of values about their mean.

326 std\_err

# Value

Return value depends on argument x. If vector, returns the standard deviation. If matrix, returns vector containing the standard deviation of each column.

#### Note

```
flag = 0 produces the same result as R's sd().
```

# **Examples**

```
std(1:10) # 3.027650
std(1:10, flag=1) # 2.872281
```

std\_err

Standard Error

# **Description**

Standard error of the values of x.

# Usage

```
std_err(x)
```

# Arguments

Х

numeric vector or matrix

#### **Details**

Standard error is computed as var(x)/length(x).

#### Value

Returns the standard error of all elements of the vector or matrix.

```
std_err(1:10) #=> 0.9574271
```

steep\_descent 327

steep_descent	Steepest Descent Minimization

# **Description**

Function minimization by steepest descent.

# Usage

# Arguments

x0	start value.
A 0	start varue.

f function to be minimized.

g gradient function of f; if NULL, a numerical gradient will be calculated.

info logical; shall information be printed on every iteration?

maxiter max. number of iterations.

tol relative tolerance, to be used as stopping rule.

#### **Details**

Steepest descent is a line search method that moves along the downhill direction.

# Value

List with following components:

xmin minimum solution found. fmin value of f at minimum.

niter number of iterations performed.

#### Note

Used some Matlab code as described in the book "Applied Numerical Analysis Using Matlab" by L. V.Fausett.

## References

Nocedal, J., and S. J. Wright (2006). Numerical Optimization. Second Edition, Springer-Verlag, New York, pp. 22 ff.

#### See Also

```
fletcher_powell
```

328 str2num

## **Examples**

```
## Rosenbrock function: The flat valley of the Rosenbruck function makes
## it infeasible for a steepest descent approach.
# rosenbrock <- function(x) {</pre>
     n \leftarrow length(x)
     x1 <- x[2:n]
      x2 <- x[1:(n-1)]
      sum(100*(x1-x2^2)^2 + (1-x2)^2)
#
# }
# steep_descent(c(1, 1), rosenbrock)
# Warning message:
# In steep_descent(c(0, 0), rosenbrock) :
   Maximum number of iterations reached -- not converged.
## Sphere function
sph \leftarrow function(x) sum(x^2)
steep_descent(rep(1, 10), sph)
        0000000000
# $xmin
# $fmin
# $niter 2
```

str2num

Converting string to number (Matlab style)

## **Description**

Functions for converting strings to numbers and numbers to strings.

# Usage

```
str2num(S)
num2str(A, fmt = 3)
```

#### **Arguments**

S string containing numbers (in Matlab format).

A numerical vector or matrix.

fmt format string, or integer indicating number of decimals.

#### **Details**

str2num converts a string containing numbers into a numerical object. The string can begin and end with '[' and ']', numbers can be separated with blanks or commas; a semicolon within the brackets indicates a new row for matrix input. When a semicolon appears behind the braces, no output is shown on the command line.

num2str converts a numerical object, vector or matrix, into a character object of the same size. fmt will be a format string for use in sprintf, or an integer n being used in '%.nf'.

streat 329

#### Value

Returns a vector or matrix of the same size, converted to strings, respectively numbers.

#### See Also

```
sprintf
```

# **Examples**

```
str1 <- " [1 2 3; 4, 5, 6; 7,8,9] "
str2num(str1)
# matrix(1:9, nrow = 3, ncol = 3, byrow = TRUE)

# str2 <- " [1 2 3; 45, 6; 7,8,9] "
# str2num(str2)
# Error in str2num(str2) :
# All rows in Argument 's' must have the same length.

A <- matrix(c(pi, 0, exp(1), 1), 2, 2)
B <- num2str(A, 2); b <- dim(B)
B <- as.numeric(B); dim(B) <- b

B
# [,1] [,2]
# [1,] 3.14 2.72
# [2,] 0.00 1.00</pre>
```

strcat

String Concatenation

# Description

Concatenate all strings in a character vector

# Usage

```
strcat(s1, s2 = NULL, collapse = "")
```

## Arguments

```
    character string or vectors
    character string or vector, or NULL (default)
    collapse
    character vector of length 1 (at best a single character)
```

#### **Details**

Concatenate all strings in character vector s1, if s2 is NULL, or cross-concatenate all string elements in s1 and s2 using collapse as 'glue'.

330 strcmp

#### Value

a character string or character vector

#### See Also

paste

# **Examples**

```
strcat(c("a", "b", "c")) #=> "abc"
strcat(c("a", "b"), c("1", "2"), collapse="x") #=> "ax1" "ax2" "bx1" "bx2"
```

strcmp

String Comparison

# **Description**

Compare two strings or character vectors for equality.

# Usage

```
strcmp(s1, s2)
strcmpi(s1, s2)
```

# Arguments

s1, s2

character strings or vectors

# **Details**

For strcmp comparisons are case-sensitive, while for strcmpi the are case-insensitive. Leading and trailing blanks do count.

#### Value

logical, i.e. TRUE if s1 and s2 have the same length as character vectors and all elements are equal as character strings, else FALSE.

## See Also

strcat

```
strcmp(c("yes", "no"), c("yes", "no"))
strcmpi(c("yes", "no"), c("Yes", "No"))
```

strfind 331

strfind

Find Substrings

# **Description**

Find substrings within strings of a character vector.

# Usage

```
strfind(s1, s2, overlap = TRUE)
strfindi(s1, s2, overlap = TRUE)
findstr(s1, s2, overlap = TRUE)
```

# Arguments

s1	character string or character vector
s2	character string (character vector of length 1)
overlap	logical (are overlapping substrings allowed)

#### **Details**

strfind finds positions of substrings within s1 that match exactly with s2, and is case sensitive; no regular patterns.

strfindi does not distinguish between lower and upper case.

findstr should only be used as internal function, in Matlab it is deprecated. It searches for the shorter string within the longer one.

# Value

Returns a vector of indices, or a list of such index vectors if s2 is a character vector of length greater than 1.

#### See Also

```
\operatorname{strcmp}
```

```
S <- c("", "ab", "aba", "aba aba", "abababa")
s <- "aba"
strfind(S, s)
strfindi(toupper(S), s)
strfind(S, s, overlap = FALSE)</pre>
```

332 strjust

strjust

Justify character vector

# Description

Justify the strings in a character vector.

#### Usage

```
strjust(s, justify = c("left", "right", "center"))
```

# **Arguments**

s Character vector.

justify Whether to justify left, right, or centered.

#### **Details**

strjust(s) or strjust(s, justify = ``right'') returns a right-justified character vector. All strings have the same length, the length of the longest string in s — but the strings in s have been trimmed before.

```
strjust(s, justify = ``left'') does the same, with all strings left-justified.
```

strjust(s, justify = ``centered'') returns all string in s centered. If an odd number of blanks has to be added, one blank more is added to the left than to the right.

# Value

A character vector of the same length.

# See Also

```
strTrim
```

```
S <- c("abc", "letters", "1", "2 2")
strjust(S, "left")</pre>
```

strrep 333

strrep

Find and replace substring

# **Description**

Find and replace all occurrences of a substring with another one in all strings of a character vector.

# Usage

```
strrep(s, old, new)
```

# **Arguments**

s Character vector.

old String to be replaced.

new String that replaces another one.

# **Details**

Replaces all occurrences of old with new in all strings of character vector s. The matching is case sensitive.

#### Value

A character vector of the same length.

#### See Also

```
gsub, regexprep
```

334 strTrim

strTrim

Remove leading and trailing white space.

# Description

Removes leading and trailing white space from a string.

# Usage

```
strTrim(s)
deblank(s)
```

# Arguments

S

character string or character vector

#### **Details**

strTrim removes leading and trailing white space from a string or from all strings in a character vector.

deblank removes trailing white space only from a string or from all strings in a character vector.

# Value

A character string or character vector with (leading and) trailing white space.

# See Also

```
strjust
```

```
s <- c(" abc", "abc ", " abc ", " a b c ", "abc", "a b c")
strTrim(s)
deblank(s)</pre>
```

subspace 335

subspace

Angle between two subspaces

# **Description**

Finds the angle between two subspaces.

# Usage

```
subspace(A, B)
```

# **Arguments**

A, B

Numeric matrices; vectors will be considered as column vectors. These matrices must have the same number or rows.

#### **Details**

Finds the angle between two subspaces specified by the columns of A and B.

# Value

An angle in radians.

#### Note

It is not necessary that two subspaces be the same size in order to find the angle between them. Geometrically, this is the angle between two hyperplanes embedded in a higher dimensional space.

# References

Strang, G. (1998). Introduction to Linear Algebra. Wellesley-Cambridge Press.

# See Also

orth

```
180 * subspace(c(1, 2), c(2, 1)) / pi #=> 36.87
180 * subspace(c(0, 1), c(1, 2)) / pi #=> 26.565

H <-
hadamard(8)
A <- H[, 2:4]
B <- H[, 5:8]
subspace(A, B) #=> 1.5708 or pi/2, i.e. A and B are orthogonal
```

336 taylor

taylor

Taylor Series Approximation

# **Description**

Local polynomial approximation through Taylor series.

# Usage

```
taylor(f, x0, n = 4, ...)
```

# **Arguments**

```
f differentiable function.

x0 point where the series expansion will take place.

n Taylor series order to be used; should be n <= 4.

... more variables to be passed to function f.
```

#### **Details**

Calculates the first four coefficients of the Taylor series through numerical differentiation and uses some polynomial 'yoga'.

# Value

Vector of length n+1 representing a polynomial of degree n.

#### Note

TODO: Pade approximation.

#### See Also

fderiv

tic,toc 337

```
yp <- polyval(p, x)
plot(x, yf, type = "1", col = "gray", lwd = 3)
lines(x, yp, col = "red")
grid()
## End(Not run)</pre>
```

tic,toc

MATLAB timer functions

# **Description**

Provides stopwatch timer. Function tic starts the timer and toc updates the elapsed time since the timer was started.

# Usage

```
tic(gcFirst=FALSE)
toc(echo=TRUE)
```

# **Arguments**

gcFirst logical scalar. If TRUE, perform garbage collection prior to starting stopwatch echo logical scalar. If TRUE, print elapsed time to screen

#### **Details**

Provides analog to system. time. Function toc can be invoked multiple times in a row.

# Value

toc invisibly returns the elapsed time as a named scalar (vector).

# Author(s)

P. Roebuck proebuck@mdanderson.org>

```
tic()
for(i in 1:100) mad(runif(1000)) # kill time
toc()
```

Toeplitz

titanium

Titanium Test Data

# **Description**

The Titanium data set describes measurements of a certain property of titanium as a function of temperature.

# Usage

```
data(titanium)
```

#### **Format**

The format is:

Two columns called 'x' and 'y', the first being the temperature.

# **Details**

These data have become a standard test for data fitting since they are hard to fit by classical techniques and have a significant amount of noise.

# Source

Boor, C. de, and J. R. Rice (1968). Least squares cubic spline approximation II – Variable knots, CSD TR 21, Comp.Sci., Purdue Univ.

# **Examples**

```
## Not run:
data(titanium)
plot(titanium)
grid()
## End(Not run)
```

Toeplitz

Toeplitz Matrix

# Description

Generate Toeplitz matrix from column and row vector.

# Usage

```
Toeplitz(a, b)
```

Trace 339

# **Arguments**

a vector that will be the first column

b vector that if present will form the first row.

#### **Details**

Toeplitz(a, b) returns a (non-symmetric) Toeplitz matrix whose first column is a and whose first row is b. The following rows are shifted to the left.

If the first element of b differs from the last element of a it is overwritten by this one (and a warning sent).

#### Value

```
Matrix of size (length(a), length(b)).
```

#### Note

stats::Toeplitz does not allow to specify the row vector, that is returns only the *symmetric* Toeplitz matrix.

#### See Also

hankel

# **Examples**

```
Toeplitz(c(1, 2, 3, 4, 5))
Toeplitz(c(1, 2, 3, 4, 5), c(1.5, 2.5, 3.5, 4.5, 5.5))
```

Trace

Matrix trace

# **Description**

Sum of the main diagonal elements.

# Usage

Trace(a)

# Arguments

а

a square matrix

#### **Details**

Sums the elements of the main diagonal of areal or complrx square matrix.

340 trapz

#### Value

scalar value

#### Note

The corresponding function in Matlab/Octave is called trace(), but this in R has a different meaning.

#### See Also

```
Diag, diag
```

# **Examples**

```
Trace(matrix(1:16, nrow=4, ncol=4))
```

trapz

Trapezoidal Integration

# **Description**

Compute the area of a function with values y at the points x.

## Usage

```
trapz(x, y)
cumtrapz(x, y)
```

# **Arguments**

x x-coordinates of points on the x-axis

y y-coordinates of function values

#### **Details**

The points (x, 0) and (x, y) are taken as vertices of a polygon and the area is computed using polyarea. This approach matches exactly the approximation for integrating the function using the trapezoidal rule with basepoints x.

cumtrapz computes the cumulative integral of y with respect to x using trapezoidal integration. x and y must be vectors of the same length, or x must be a vector and y a matrix whose first dimension is length(x).

Inputs x and y can be complex.

#### Value

Approximated integral of the function from min(x) to max(x). Or a matrix of the same size as y.

tri 341

## See Also

```
polyarea
```

# **Examples**

```
# Calculate the area under the sine curve from 0 to pi:
n <- 101
x <- seq(0, pi, len = n)
y \leftarrow sin(x)
trapz(x, y)
                                   #=> 1.999835504
# Use a correction term at the boundary: -h^2/12*(f'(b)-f'(a))
h <- x[2] - x[1]
ca <- (y[2]-y[1]) / h
cb <- (y[n]-y[n-1]) / h
trapz(x, y) - h^2/12 * (cb - ca) #=> 1.999999969
# Use two complex inputs
z <- exp(1i*pi*(0:100)/100)
ct <- cumtrapz(z, 1/z)</pre>
                                   #=> 0+3.14107591i
ct[101]
```

tri

Triangular Matrices (Matlab Style)

# Description

Extract lower or upper triangular part of a matrix.

# Usage

```
tril(M, k = 0)

triu(M, k = 0)
```

#### **Arguments**

M numeric matrix.

k integer, indicating a secondary diagonal.

#### **Details**

tril

Returns the elements on and below the kth diagonal of X, where k = 0 is the main diagonal, k > 0 is above the main diagonal, and k < 0 is below the main diagonal.

triu

Returns the elements on and above the kth diagonal of X, where k = 0 is the main diagonal, k > 0 is above the main diagonal, and k < 0 is below the main diagonal.

342 trigApprox

# Value

Matrix the same size as the input matrix.

#### Note

For k==0 it is simply an application of the R functions lower.tri resp. upper.tri.

# See Also

Diag

# **Examples**

```
tril(ones(4,4), +1)
# 1 1 0 0
# 1 1 1 0
# 1 1 1 1
# 1 1 1 1

triu(ones(4,4), -1)
# 1 1 1 1
# 0 1 1 1
# 0 0 1 1
```

trigApprox

Trigonometric Approximation

# Description

Computes the trigonometric series.

# Usage

```
trigApprox(t, x, m)
```

# Arguments

```
t vector of points at which to compute the values of the trigonometric approximation.

Adata from t=0 to t=2*(n-1)*pi/n
```

x data from t=0 to t=2\*(n-1)\*pi/n.

m degree of trigonometric regression.

# **Details**

Calls trigPoly to get the trigonometric coefficients and then sums the finite series.

trigPoly 343

#### Value

Vector of values the same length as t.

#### Note

TODO: Return an approximating function instead.

# See Also

```
trigPoly
```

# **Examples**

```
## Not run:
## Example: Gauss' Pallas data (1801)
asc <- seq(0, 330, by = 30)
dec <- c(408, 89, -66, 10, 338, 807, 1238, 1511, 1583, 1462, 1183, 804)
plot(2*pi*asc/360, dec, pch = "+", col = "red", xlim = c(0, 2*pi), ylim = c(-500, 2000),
     xlab = "Ascension [radians]", ylab = "Declination [minutes]",
     main = "Gauss' Pallas Data")
grid()
points(2*pi*asc/360, dec, pch = "o", col = "red")
ts <- seq(0, 2*pi, len = 100)
xs <- trigApprox(ts ,dec, 1)</pre>
lines(ts, xs, col = "black")
xs <- trigApprox(ts ,dec, 2)</pre>
lines(ts, xs, col = "blue")
legend(3, 0, c("Trig. Regression of degree 1", "Trig. Regression of degree 2",
                  "Astronomical position"), col = c("black", "blue", "red"),
                lty = c(1,1,0), pch = c("", "", "+"))
## End(Not run)
```

trigPoly

Trigonometric Polynomial

# Description

Computes the trigonometric coefficients.

## Usage

```
trigPoly(x, m)
```

# Arguments

```
x data from t=0 to t=2*(n-1)*pi/n.
m degree of trigonometric regression.
```

344 trigPoly

#### **Details**

Compute the coefficients of the trigonometric series of degree m,

$$a_0 + \sum_k (a_k \cos(kt) + b_k \sin(kt))$$

by applying orthogonality relations.

#### Value

Coefficients as a list with components a0, a, and b.

#### Note

For irregular spaced data or data not covering the whole period, use standard regression techniques, see examples.

#### References

Fausett, L. V. (2007). Applied Numerical Analysis Using Matlab. Second edition, Prentice Hall.

#### See Also

trigApprox

```
# Data available only from 0 to pi/2
t <- seq(0, pi, len=7)
x <- 0.5 + 0.25*sin(t) + 1/3*cos(t) - 1/3*sin(2*t) - 0.25*cos(2*t)
# use standard regression techniques
A \leftarrow cbind(1, cos(t), sin(t), cos(2*t), sin(2*t))
ab <- qr.solve(A, x)
# [1] 0.5000000 0.3333333 0.2500000 -0.2500000 -0.3333333
ts \leftarrow seq(0, 2*pi, length.out = 100)
xs <- ab[1] + ab[2]*cos(ts) +
      ab[3]*sin(ts) + ab[4]*cos(2*ts) + ab[5]*sin(2*ts)
## Not run:
# plot to make sure
plot(t, x, col = "red", xlim=c(0, 2*pi), ylim=c(-2,2),
           main = "Trigonometric Regression")
lines(ts, xs, col="blue")
grid()
## End(Not run)
```

triquad 345

triquad	Gaussian Triangle Quadrature	

#### **Description**

Numerically integrates a function over an arbitrary triangular domain by computing the Gauss nodes and weights.

## Usage

```
triquad(f, x, y, n = 10, tol = 1e-10, ...)
```

# Arguments

f	the integrand as function of two variables.
x	x-coordinates of the three vertices of the triangle.
у	y-coordinates of the three vertices of the triangle.
n	number of nodes.
tol	relative tolerance to be achieved.
	additional parameters to be passed to the function.

# **Details**

Computes the N^2 nodes and weights for a triangle with vertices given by 3x2 vector. The nodes are produced by collapsing the square to a triangle.

Then f will be applied to the nodes and the result multiplied left and right with the weights (i.e., Gaussian quadrature).

By default, the function applies Gaussian quadrature with number of nodes n=10,21,43,87,175 until the relative error is smaller than the tolerance.

#### Value

The integral as a scalar.

#### Note

A small relative tolerance is *not* really indicating a small absolute tolerance.

# Author(s)

Copyright (c) 2005 Greg von Winckel Matlab code based on the publication mentioned and available from MatlabCentral (calculates nodes and weights). Translated to R (with permission) by Hans W Borchers.

346 trisolve

#### References

Lyness, J. N., and R. Cools (1994). A Survey of Numerical Cubature over Triangles. Proceedings of the AMS Conference "Mathematics of Computation 1943–1993", Vancouver, CA.

#### See Also

```
quad2d, simpson2d
```

## **Examples**

trisolve

Tridiagonal Linear System Solver

## **Description**

Solves tridiagonal linear systems A\*x=rhs efficiently.

#### Usage

```
trisolve(a, b, d, rhs)
```

#### Arguments

```
    a diagonal of the tridiagonal matrix A.
    b, d upper and lower secondary diagonal of A.
    rhs right hand side of the linear system A*x=rhs.
```

## **Details**

Solves tridiagonal linear systems A\*x=rhs by applying Givens transformations.

By only storing the three diagonals, trisolve has memory requirements of 3\*n instead of n^2 and is faster than the standard solve function for larger matrices.

vander 347

#### Value

Returns the solution of the tridiagonal linear system as vector.

#### Note

Has applications for spline approximations and for solving boundary value problems (ordinary differential equations).

#### References

Gander, W. (1992). Computermathematik. Birkhaeuser Verlag, Basel.

#### See Also

```
qrSolve
```

# **Examples**

```
set.seed(8237)
a <- rep(1, 100)
e <- runif(99); f <- rnorm(99)
x <- rep(seq(0.1, 0.9, by = 0.2), times = 20)
A <- diag(100) + Diag(e, 1) + Diag(f, -1)
rhs <- A %*% x
s <- trisolve(a, e, f, rhs)
s[1:10]  #=> 0.1 0.3 0.5 0.7 0.9 0.1 0.3 0.5 0.7 0.9
s[91:100]  #=> 0.1 0.3 0.5 0.7 0.9 0.1 0.3 0.5 0.7 0.9
```

vander

Vandermonde matrix

# Description

Generate Vandermonde matrix from a numeric vector.

# Usage

```
vander(x)
```

# **Arguments**

Х

Numeric vector

#### **Details**

Generates the usual Vandermonde matrix from a numeric vector, e.g. applied when fitting a polynomial to given points. Complex values are allowed.

348 vectorfield

# Value

Vandermonde matrix of dimension n where n = length(x).

# **Examples**

```
vander(c(1:10))
```

vectorfield

Vector Field Plotting

# Description

Plotting a vector field

# Usage

# Arguments

fun	function of two variables — must be vectorized.
xlim	range of x values.
ylim	range of y values.
n	grid size, proposed 16 in each direction.
scale	scales the length of the arrows.
col	arrow color, proposed 'green'.
	more options presented to the arrows primitive.

# **Details**

Plots a vector field for a function f. Main usage could be to plot the solution of a differential equation into the same graph.

# Value

Opens a graph window and plots the vector field.

# See Also

```
quiver, arrows
```

whittaker 349

#### **Examples**

```
f <- function(x, y) x^2 - y^2
xx <- c(-1, 1); yy <- c(-1, 1)
## Not run:
vectorfield(f, xx, yy, scale = 0.1)
for (xs in seq(-1, 1, by = 0.25)) {
    sol <- rk4(f, -1, 1, xs, 100)
        lines(sol$x, sol$y, col="darkgreen")
}
grid()
## End(Not run)</pre>
```

whittaker

Whittaker Smoothing

#### **Description**

Smoothing of time series using the Whittaker-Henderson approach.

#### Usage

```
whittaker(y, lambda = 1600, d = 2)
```

#### **Arguments**

y signal to be smoothed.

lambda smoothing parameter (rough 50..1e4 smooth); the default value of 1600 has been

recommended in the literature.

d order of differences in penalty (generally 2)

# Details

The Whittaker smoother family was first presented by Whittaker in 1923 for life tables, based on penalized least squares. These ideas were revived by Paul Eilers, Leiden University, in 2003. This approach is also known as Whittaker-Henderson smoothing.

The smoother attempts to both fit a curve that represents the raw data, but is penalized if subsequent points vary too much. Mathematically it is a large, but sparse optimization problem that can be expressed in a few lines of Matlab or R code.

#### Value

A smoothed time series.

#### Note

```
*** The function is not yet fully implemented ***
```

See the example in 'savgol' for working code. This R implementation requires the SparseM package. It will stop if this package cannot be loaded.

350 wilkinson

#### Author(s)

An R version, based on Matlab code by P. Eilers in 2002, has been published by Nicholas Lewin-Koh on the R-help mailing list in February 2004, and in private communication to the author of this package.

#### References

P. H. C. Eilers (2003). A Perfect Smoother. Analytical Chemistry, Vol. 75, No. 14, pp. 3631–3636. Wilson, D. I. (2006). The Black Art of Smoothing. Electrical and Automation Technology, June/July issue.

#### See Also

```
savgol, ptw::whit2
```

# **Examples**

```
## Not run:
# *** Sinosoid test function ***
ts <- sin(2*pi*(1:1000)/200)
t1 <- ts + rnorm(1000)/10
t3 <- whittaker(t1, lambda = 1000)
plot(1:1000, t1, col = "grey")
lines(1:1000, ts, col="blue")
lines(1:1000, t3, col="red")
## End(Not run)</pre>
```

wilkinson

wilkinson Matrix

# **Description**

Generate the Wilkinson matrix of size n x n.The Wilkinson matrix for testing eigenvalue computations

# Usage

```
wilkinson(n)
```

# **Arguments**

n

integer

#### **Details**

The Wilkinson matrix for testing eigenvalue computations is a symmetric matrix with three non-zero diagonals and with several pairs of nearly equal eigenvalues.

zeta 351

#### Value

```
matrix of size n x n
```

#### Note

The two largest eigenvalues of wilkinson(21) agree to 14, but not 15 decimal places.

#### See Also

```
Toeplitz
```

#### **Examples**

```
(a <- wilkinson(7))
eig(a)</pre>
```

zeta

Riemann Zeta Function

# **Description**

Riemann's zeta function valid in the entire complex plane.

#### Usage

```
zeta(z)
```

# Arguments

Z

Real or complex number or a numeric or complex vector.

# **Details**

Computes the zeta function for complex arguments using a series expansion for Dirichlet's eta function.

Accuracy is about 13 significant digits for abs(z)<100, drops off with higher absolute values.

#### Value

Returns a complex vector of function values.

# Note

Copyright (c) 2001 Paul Godfrey for a Matlab version available on Mathwork's Matlab Central under BSD license.

#### References

Zhang, Sh., and J. Jin (1996). Computation of Special Functions. Wiley-Interscience, New York.

352 zeta

#### See Also

```
gammaz, eta
```

```
## First zero on the critical line s = 0.5 + i t
x <- seq(0, 20, len=1001)
z <- 0.5 + x*1i
fr <- Re(zeta(z))</pre>
fi <- Im(zeta(z))</pre>
fa <- abs(zeta(z))</pre>
plot(x, fa, type="n", xlim = c(0, 20), ylim = c(-1.5, 2.5),
     xlab = "Imaginary part (on critical line)", ylab = "Function value",
     main = "Riemann's Zeta Function along the critical line")
lines(x, fr, col="blue")
lines(x, fi, col="darkgreen")
lines(x, fa, col = "red", lwd = 2)
points(14.1347, 0, col = "darkred")
legend(0, 2.4, c("real part", "imaginary part", "absolute value"),
       lty = 1, lwd = c(1, 1, 2), col = c("blue", "darkgreen", "red"))
grid()
## End(Not run)
```

# **Index**

*Topic <b>arith</b>	inv, 167
agmean, 14	itersolve, 172
angle, 20	kron, 175
bits, 29	lu, 195
ceil, 42	magic, 197
combs, 51	meshgrid, 198
eps, 83	moler, 204
gcd, 1cm, 129	ndims, 209
invperm, 169	nearest_spd, 210
mod, rem, 202	nnz, 222
nchoosek, 208	Norm, 223
nextpow2, 220	normest, 224
nthroot, 225	nullspace, 226
perms, 239	nume1, 228
pow2, 257	orth, 234
primes, 261	pinv, 241
randcomb, 280	poly2str, 245
randperm, 281	procrustes, 262
*Topic <b>array</b>	qrSolve, 266
accumarray, 12	Rank, 282
blkdiag, 31	repmat, 291
charpoly, 43	Reshape, 292
compan, 51	rosser, 301
cond, 54	size, 315
cross, 61	sorting, 317
crossn, 62	sortrows, 319
Diag, 73	squareform, 324
distmat, 76	subspace, 335
dot, 78	Toeplitz, 338
eig, 78	Trace, 339
eye, <mark>92</mark>	tri,341
givens, 132	trisolve, 346
gramSchmidt, 138	vander, 347
hadamard, 139	wilkinson, 350
hankel, 142	*Topic datasets
hilb, 145	brown72, 33
householder, 151	nile, 221
hypot, 155	titanium, 338
ifft, 156	*Topic <b>fitting</b>

al imates and 17	h 25
akimaInterp, 17	barylag, 25
circlefit, 47	barylag2d, 26
cubicspline, 63	bisect, 28
curvefit, 64	brentDekker, 32
fornberg, 113	broyden, 34
kriging, 174	bsxfun, 35
lsqlin, 190	cart2sph, 40
lsqnonlin, 192	chebApprox, 44
mexpfit, 199	chebCoeff, 45
odregress, 232	chebPoly, 46
ppfit, 258	clenshaw_curtis, 50
ppval, 259	complexstep, 52
ratinterp, 284	cot,csc,sec, etc.,56
rationalfit, 285	cotes, 57
*Topic <b>geom</b>	coth,csch,sech, etc.,58
inpolygon, 157	dblquad, 67
segm_distance, 308	deg2rad, 71
segm_intersect, 309	detrend, 71
*Topic graphs	eigjacobi, 79
andrewsplot, 19	ellipke,ellipj,82
errorbar, 85	eta, 86
ezcontour, ezmesh, 92	expint, 88
ezplot, 94	expm, 90
ezpolar, 95	fact, 96
figure, 100	factors, 97
fplot, 114	fderiv, 98
peaks, 238	findzeros, 105
plotyy, 242	fnorm, 112
polar, 243	fresnelS/C, 115
quiver, 277	fzero, 118
semilogx, semilogy, 311	fzsolve, 119
vectorfield, 348	gammainc, 120
*Topic <b>logic</b>	gammaz, 121
and, or, 18	gauss_kronrod, 128
findintervals, 101	gaussHermite, 122
finds, 104	gaussLaguerre, 124
isempty, 170	gaussLegendre, 125
*Topic <b>manip</b>	gaussNewton, 126
flipdim, 108	gmres, 133
histc, 146	grad, 136
linspace, 188	gradient, 137
logspace, 189	halley, 140
Mode, 203	hausdorff_dist, 143
rot90, 302	hessian, 144
str2num, 328	horner, 150
*Topic <b>math</b>	integral, 159
aitken, 16	integral2, 161
arclength, 23	interp1, 163
ai cicliguii, 23	πιτοι μ1, 103

interp2, 165	runge, 304
isprime, 171	simpadpt, 313
jacobian, 173	simpson2d, 314
laguerre, 178	spinterp, 320
lambertWp, 179	sqrtm, rootm, 322
laplacian, 180	taylor, 336
lebesgue, 182	trapz, 340
legendre, 183	trigApprox,342
line_integral, 184	trigPoly,343
mldivide, 201	triquad, 345
muller, 207	zeta, 351
neville, 213	*Topic <b>ode</b>
newtonHorner, 215	abm3pc, <u>11</u>
newtonInterp, 216	bulirsch-stoer, 36
newtonRaphson, 217	bvp, 38
newtonsys, 219	cranknic, 59
numderiv, 227	deeve, 70
pade, 235	deval, 72
pascal, 236	euler_heun, 87
pchip, 237	newmark, 214
piecewise, 240	ode23, <u>229</u>
Poly, 244	rk4, rk4sys, <u>295</u>
polyadd, 245	rkf54, 296
polyApprox, 246	*Topic <b>optimize</b>
polyarea, 247	direct1d,74
polyder, 250	fibsearch, 99
polyfit, 251	findmins, 102
polyint, 252	fletcher-powell, 106
polylog, 253	fminbnd, 109
polymul, 254	fminsearch, 110
polypow, 255	fsolve, 117
polytrans, 256	geo_median, 131
polyval, 257	golden_ratio, 135
quad, 267	hooke_jeeves, 148
quad2d, 269	L1linreg, 176
quadcc, 270	linprog, 185
quadgk, 271	nelder_mead, 211
quadgr, 272	softline, 316
quadinf, 273	steep_descent, 327
quad1, 274	*Topic <b>package</b>
quadv, 275	pracma-package, 8
rat, 283	*Topic <b>stat</b>
rectint, 287	erf, 84
ridders, 292	geomean, harmmean, 130
romberg, 299	rand, 278
roots, 300	rmserr, 298
rortho, 301	runs.test, 305
rref, 303	std, 325

std_err, 326	asech (coth,csch,sech, etc.), 58
*Topic <b>string</b>	
blanks, 30	barylag, 25, 27, 182, 213, 217
refindall, 288	barylag2d, 26, <i>175</i>
regexp, 289	beep (disp, beep), 76
regexprep, 290	bisect, 28
strcat, 329	bits, 29
strcmp, 330	blanks, 30
strfind, 331	blkdiag, 31
strjust, 332	brent, <i>119</i> , <i>293</i>
strrep, 333	brent (brentDekker), 32
strTrim, 334	brentDekker, 32
*Topic <b>timeseries</b>	brown72, 33
approx_entropy, 21	broyden, 34, 118, 219
conv, 55	bsxfun, 35
cutpoints, 66	<pre>bubbleSort(sorting), 317</pre>
deconv, 69	bulirsch-stoer, 36
findpeaks, 103	bulirsch_stoer(bulirsch-stoer), 36
hampel, 141	bvp, 38
histss, 147	
hurstexp, 153	cart2pol (cart2sph), 40
invlap, 168	cart2sph, $40$
movavg, 205	cd(cd, pwd, what), 41
savgol, 306	cd, pwd, what,41
whittaker, 349	ceil, 42
*Topic utilities	charpoly, 43
disp, beep, 76	chebApprox, 44, 46, 47, 247
tic, toc, 337	chebCoeff, 45, 47
• •	chebPoly, 46, 46, 183
abm3pc, 11	chisq.test, 306
abs, <i>21</i>	choose, 209
accumarray, 12	circlefit, 47, <i>65</i>
acot(cot,csc,sec, etc.),56	circshift (flipdim), 108
acoth(coth,csch,sech, etc.),58	clear(clear, who(s), ver),49
acsc(cot,csc,sec, etc.),56	clear, who(s), ver,49
acsch(coth,csch,sech, etc.),58	clenshaw_curtis,50
agmean, 14	combs, 51, 280
aitken, 16	compan, 51, 79
akimaInterp, 17, 175	complexstep, 52, 228
and (and, or), 18	cond, 54, 225
and, or, 18	contour, 93
andrewsplot, 19	conv, 55, 69, 246
angle, 20	cot(cot,csc,sec, etc.),56
approx, 164	cot,csc,sec, etc.,56
approx_entropy, 21	cotes, 57
arclength, 23, 248	coth(coth,csch,sech, etc.),58
arrayfun (bsxfun), 35	coth,csch,sech, etc.,58
arrows, 277, 348	cranknic, 59, 88, 215
asec (cot,csc,sec, etc.), 56	cross, 61, 62, 78

crossn, 61, 62	eye, 92
csc(cot,csc,sec, etc.),56	ezcontour (ezcontour, ezmesh), 92
csch (coth,csch, sech, etc.), 58	ezcontour, ezmesh, 92
cubicspline, 63, 260	ezmesh (ezcontour, ezmesh), 92
cumtrapz (trapz), 340	ezplot, 94, 96
curve, <i>95</i>	ezpolar, 95
curvefit, 64	
cut, <i>67</i>	fact, 96
cutpoints, 66	factorial, 96
	factors, 97, <i>171</i> , <i>261</i>
dblquad, 67, <i>315</i>	fderiv, 98, <i>136</i> , <i>137</i> , <i>228</i> , <i>336</i>
deblank, 30	fft, <i>157</i>
deblank (strTrim), 334	fftshift (ifft), 156
deconv, 56, 69	fibsearch, 99, 110
deeve, 70, <i>73</i>	figure, 100
deg2rad, 71	find, 223
detrend, 71	findInterval, <i>146</i>
deval, 70, 72, 230, 295	findintervals, 101
Diag, 31, 73, 92, 340, 342	findmins, 75, 102, 105
diag, 74, 340	findpeaks, 103, <i>142</i>
dim, <i>316</i>	finds, 104
direct1d, 74	findstr (strfind), 331
disp (disp, beep), 76	findzeros, 105
disp, beep, 76	Fix (ceil), 42
dist, 77, 325	fletcher-powell, 106
distmat, 76, 144	fletcher_powell, 327
dot, 61, 62, 78	fletcher_powell(fletcher-powell), 106
	flipdim, 108
eig, 78, <i>80</i>	fliplr (flipdim), 108
eigjacobi, 79	flipud (flipdim), 108
einsteinF, 80	fminbnd, 109
ellipj(ellipke,ellipj),82	fminsearch, 110
ellipke(ellipke,ellipj),82	fnorm, 112, 305
ellipke,ellipj,82	fornberg, 113
eps, 83	fplot, 114
erf, 84	fresnelC (fresnelS/C), 115
erfc (erf), 84	fresnelS (fresnelS/C), 115
erfcinv(erf), 84	fresnelS/C, 115
erfcx (erf), 84	fsolve, <i>34</i> , 117
erfi (erf), 84	fzero, 118
erfinv(erf),84	fzsolve, 119
erfz (erf), 84	
errorbar, 85	gamma, <i>121</i> , <i>122</i>
eta, 86, <i>352</i>	gammainc, 120
euler_heun, 87	gammaz, 87, 121, 352
expint, 88	gauss_kronrod, <i>50</i> , 128
expint_E1 (expint), 88	gaussHermite, 122, <i>125</i> , <i>126</i>
expint_Ei (expint), 88	gaussLaguerre, 123, 124, 126
expm, 90, 324	gaussLegendre, 50, 116, 123, 125, 125

gaussNewton, 118, 126, 317	interp2, 27, 165
gcd (gcd, 1cm), 129	inv, 167
gcd, 1cm, 129	invlap, 168
geo_median, 131	invperm, 169
_	
geomean (geomean, harmmean), 130	is.sorted(sorting), 317
geomean, harmmean, 130	isempty, 170
getwd, <i>41</i>	isprime, <i>97</i> , 171, <i>261</i>
givens, 132, <i>139</i> , <i>152</i>	itersolve, 172
gmres, 133	
golden_ratio, <i>110</i> , 135	jacobian, 173
grad, 136	<pre>jacobian_csd(complexstep), 52</pre>
<pre>grad_csd (complexstep), 52</pre>	
gradient, 137	kabsch (procrustes), 262
gramSchmidt, 138	kriging, 18, 174
gsub, 290, 333	kron, 175
gsub, 290, 333	W 911, 173
hadamard, 139, <i>143</i>	L1linreg, <i>132</i> , 176
halley, 140, <i>180</i>	lagrangeInterp (newtonInterp), 216
hampel, <i>104</i> , 141	laguerre, 178
hankel, <i>140</i> , 142, <i>339</i>	lambertWn (lambertWp), 179
	lambertWp, <i>16</i> , 179
harmmean (geomean, harmmean), 130	laplacian, 145, 180
hausdorff_dist, 143	laplacian_csd (complexstep), 52
heapSort (sorting), 317	
hessian, 144, <i>181</i>	Lcm (gcd, 1cm), 129
hessian_csd (complexstep), 52	lebesgue, 182
hilb, 145	legendre, 183
hist, <i>146</i> , <i>148</i>	li (expint), 88
histc, 146, <i>148</i>	line_integral, 184
histss, <i>146</i> , 147	linprog, 185
hooke_jeeves, 148, 212	linspace, 188
horner, 150	list.files, 41
hornerdefl (horner), 150	lm, 177, 233
householder, <i>133</i> , <i>139</i> , 151, 267	logit (sigmoid), 312
humps, 152	loglog (semilogx, semilogy), 311
	logm (expm), 90
hurstexp, 153	logseq (logspace), 189
hypot, 155	
idiaida (mada mam) 202	logspace, 188, 189, 189
idivide (mod, rem), 202	ls, 49
ifft, 156	lsqcurvefit (lsqnonlin), 192
ifftshift (ifft), 156	lsqlin, <i>65</i> , 190
Imag (angle), 20	lsqnonlin, <i>177</i> , 192, <i>200</i>
image, $93$	lsqnonneg (lsqnonlin), 192
inpolygon, 157	lsqsep, 200
<pre>insertionSort (sorting), 317</pre>	lsqsep (lsqnonlin), 192
integral, 159, <i>162</i> , <i>184</i>	lu, 195
integral 2, 161	lufact (lu), 195
integral3 (integral2), 161	lusys (lu), 195
integrate, 68, 268, 274, 300	1u3y3 (1u), 17J
_	magic 107
interp1, 163, <i>166</i> , <i>237</i>	magic, 197

matlab, 198	ode23, 12, 37, 60, 215, 229, 295, 297
matplot, <i>115</i>	ode23s, <i>37</i>
mean, <i>131</i>	ode23s (ode23), 229
median, 204	ode45 (ode23), 229
mergeOrdered (sorting), 317	ode78 (ode23), 229
mergeSort (sorting), 317	odregress, 232
meshgrid, 198, 239	ones (eye), 92
mexpfit, 199	optim, <i>111</i>
midpoint (bulirsch-stoer), 36	optimize, 102
mkpp, 259	or (and, or), 18
mkpp (ppval), 259	orth, 226, 234, 335
mldivide, 201	outer, <i>199</i>
Mod, 21	,
mod (mod, rem), 202	pade, 235, 284
mod, rem, 202	pascal, 236
Mode, 203	paste, <i>330</i>
moler, 204	pchip, 237
	pchipfun (pchip), 237
movavg, 205	pdist (distmat), 76
mrdivide (mldivide), 201	pdist2 (distmat), 76
muller, 207	peaks, 238
	perms, 51, 239, 281
nchoosek, 208	persp, <i>93</i>
ndims, 209	piecewise, 240
nearest_spd, 210	pinv, 190, 241
nelder_mead, <i>149</i> , 211	plot, <i>311</i>
neville, <i>114</i> , 213, <i>217</i>	plotyy, 242
newmark, 39, 60, 214	pnorm, 85
newton (newtonRaphson), 217	pol2cart (cart2sph), 40
newtonHorner, 215, 218	polar, 20, 243
newtonInterp, <i>114</i> , <i>213</i> , 216	Poly, 244
newtonRaphson, 32, 141, 207, 216, 217, 219	poly, 251, 257
newtonsys, <i>34</i> , <i>120</i> , <i>127</i> , <i>207</i> , 219	poly2str, 245
nextpow2, <i>30</i> , 220, 258	poly_center (polyarea), 247
nile, 221	poly_crossings (polyarea), 247
nlm, <i>194</i>	poly_length, 24
nls, <i>194</i>	poly_length (polyarea), 247
nnz, 222	polyadd, <i>56</i> , 245
Norm, 112, 223	polyApprox, <i>44</i> , 246
norm, 223	polyarea, 247, 287, 341
normest, 55, 224	polyder, 250, 252
normest2 (normest), 224	polyfit, 72, 247, 251
nthroot, 225	polyfit2 (polyfit), 251
null (nullspace), 226	polygon, <i>158</i>
nullspace, 190, 226, 234, 282	polyint, 250, 252
num2str (str2num), 328	polylog, 253
numderiv, <i>53</i> , <i>99</i> , 227	polymul, 69, 254, 255
numdiff(numderiv), 227	polypow, 255, 256
numel, 228	polyroot, 300

polytrans, 256	regulaFalsi (bisect), 28
polyval, 151, 244, 250–252, 257	rem (mod, rem), 202
pow2, 221, 257	repmat, 291
ppfit, 258	Reshape, <i>291</i> , 292
ppval, 259, 259	ridders, 29, 32, 292
pracma (pracma-package), 8	rk4, 12, 297
pracma-package, 8	rk4 (rk4, rk4sys), 295
primes, 89, 97, 171, 261	rk4, rk4sys, 294
procrustes, 210, 262	rk4sys, 230
psi, 264	rk4sys (rk4, rk4sys), 295
pwd (cd, pwd, what), 41	rkf54, 296
F ( ) F	rm, 49
qpspecial, 265	rmserr, 298
qr, 196	romberg, 129, 160, 299
qr.solve, <i>303</i>	rootm (sqrtm, rootm), 322
qrSolve, 172, 266, 347	roots, 52, 178, 244, 257, 300
quad, 267, 270, 275, 276, 313	rortho, 210, 301
quad2d, 68, 269, 315, 346	rosser, 301
quadcc, 270	rot90, 302
quadgk, 129, 160, 271, 274	rref, 303
quadgr, 160, 272, 300	runge, 304
quadinf, 160, 273	runs.test, 305
quad1, 268, 274	
quadv, 160, 275	<pre>sample_entropy (approx_entropy), 21</pre>
quickSort (sorting), 317	savgol, 306, <i>350</i>
quickSortx (sorting), 317	sec(cot,csc,sec, etc.),56
quiver, 277, 348	secant, 207
	secant (newtonRaphson), 217
rad2deg (deg2rad), 71	sech(coth,csch,sech, etc.),58
rand, 278	segm_distance, 308, <i>310</i>
randcomb, <i>51</i> , 280	segm_intersect, <i>309</i> , <i>309</i>
randi (rand), 278	selectionSort(sorting), 317
randn (rand), 278	<pre>semilogx(semilogx, semilogy), 311</pre>
randp (rand), 278	semilogx, semilogy, 311
randperm, 170, 239, 280, 281	<pre>semilogy(semilogx, semilogy), 311</pre>
rands (rand), 278	seq, 188, 189
randsample (rand), 278	sessionInfo,49
Rank, 226, 282	set.seed, <i>279</i>
rat, 283	setwd, 41
ratinterp, 284, 286	shellSort (sorting), 317
rationalfit, 284, 285	sigmoid, 312
rats (rat), 283	signm (sqrtm, rootm), 322
Real (angle), 20	simpadpt, 58, 160, 313
rectint, 287	simpson2d, 68, 313, 314, 346
refindall, 288	sinc (humps), 152
regexp, 288, 289	size, 209, 229, 315
regexpi (regexp), 289	softline, 127, 316
regexpr, 289	solve, 134, 167
regexprep, 290	sort, <i>319</i>

sorting, 317	vander, <i>145</i> , 347
sortrows, 319	vectorfield, 277, 348
sph2cart (cart2sph), 40	Vectorize, 36
spinterp, 320	ver(clear, who(s), ver), 49
spline, 63, 164	
sprintf, 329	what(cd, pwd, what),41
sqrt, 225	whittaker, <i>307</i> , 349
sqrtm(sqrtm,rootm), 322	who (clear, who(s), ver), $49$
sqrtm, rootm, 322	whos (clear, who(s), ver), $49$
squareform, 324	wilkinson, <i>205</i> , <i>302</i> , <i>350</i>
std, 325	4
std_err, 326	zeros (eye), 92
steep_descent, 107, 327	zeta, <i>87</i> , 351
str2num, 328	
strcat, 329, 330	
strcmp, 330, 331	
strcmpi (strcmp), 330	
strfind, 331	
strfindi (strfind), 331	
strjust, 332, 334	
strrep, 333	
strTrim, 332, 334	
subspace, 335	
svd, 55, 225, 263	
system.time, 337	
taylor, 99, 235, 336	
testSort (sorting), 317	
tic (tic, toc), 337	
tic, toc, 337	
titanium, 338	
toc (tic, toc), 337	
Toeplitz, 140, 143, 338, 351	
Trace, 74, 339	
trapz, 58, 240, 248, 340	
tri, 341	
trigApprox, 342, 344	
trigPoly, <i>343</i> , 343	
tril (tri), 341	
trimmean (geomean, harmmean), 130	
triplequad (dblquad), 67	
triquad, 345	
trisolve, 346	
triu(tri), 341	
•	
uniq (accumarray), 12	
unique, <i>13</i>	
uniroot, 100, 119, 135	