# Manual for Package: mathematics Revision 2:9M

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### March 28, 2020

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### 1 calendar

# $1.1 \quad days\_per\_month$

### 1.2 isnight

#### 2 mathematics

mathematical functions of various kind

#### 2.1 cast\_byte\_to\_integer

cast byte to integer

### 3 complex-analysis

operations on complex numbers

#### 3.1 complex\_exp\_product\_im\_im

#### 3.2 complex\_exp\_product\_im\_re

```
product of the imaginary part of one and the real part of a second
complex exponential
the product has two frequency components
```

input :

c : complex amplitudes

o : frequencies

output :

cp : amplitude of the product
op : frequencies of the product

#### 3.3 complex\_exp\_product\_re\_im

#### $3.4 \quad complex\_exp\_product\_re\_re$

#### 3.5 croots

```
nth-roots of a complex number
input:
c : complex number
n : order of root
    n must be rational, to obtain n solutions
    otherwise no finite set of solutions exists
r : roots of the complex number
```

3.6	${f root\_complex}$
root	of a complex number
3.7	$test\_imroots$
4	derivation
deriva	ation of several functions by means of symbolic computation
4.1	derive_acfar1
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4.3	derive_arc_length
4.4	derive_fourier_power
4.5	derive_fourier_power_exp
4.6	derive_laplacian_curvilinear
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derive\_fdm\_taylor

 $derive\_fdm\_vargrid$ 

5.6

5.7

5.8 derive\_fem\_2d\_mass 5.9 derive\_fem\_error\_2d 5.10 derive\_fem\_error\_3d 5.11  $derive\_fem\_sym\_2d$ 5.12 derive\_grid\_constants 5.13 derive\_interpolation 5.14 derive\_laplacian 5.15 derive\_limit 5.16 derive\_nc\_1d

5.17 derive\_nc\_1d\_

5.18	derive_nc_2d
5.19	$derive\_nonuniform\_symmetric$
%	
5.20	$\operatorname{derive\_richardson}$
5.21	$\operatorname{derive\_sum}$
5.22	nn
5.23	${\it test\_derive}$
5.24	$test\_derive\_fdm\_poly$
5.25	${ m test\_filter}$

5.26 test\_vargrid

# 6 derivation

derivation of several functions by means of symbolic computation

# 6.1 simplify\_atan

symbolic simplification of the arcus tangent

# 7 mathematics

mathematical functions of various kind

 $7.1 \quad \exp 10$ 

# 8 finance

- $8.1 \quad derive\_skewrnd\_walsh\_paramter$
- $8.2 \quad gbm\_cdf$
- $8.3~\mathrm{gbm\_fit}$
- $8.4~gbm\_fit\_old$
- $8.5 \quad \text{gbm\_inv}$

8.6 gbm\_mean 8.7 gbm\_median  $8.8 \text{ gbm\_pdf}$  $8.9 \quad gbm\_simulate$ 8.10 gbm\_skewness  $8.11 \quad gbm\_std$  $8.12 \quad gbm\_transform\_time\_step$ 8.13 put\_price\_black\_scholes 8.14 skewgbm\_simulate

8.15 skewrnd\_walsh

- 9 finance/test
- $9.1 ext{test\_gbm}$
- 9.2  $test\_gbm\_pdf$
- 9.3 test\_skewrnd\_walsh
- 10 fourier/@STFT
- 10.1 STFT

class for short time fourier transform

Note: the interval Ti should be set to at leat 2\*max(T), as
 otherwise coefficients
 tend to oscillate in the presence of noise
Note: for convenience, the independent variable is labeled as time
 (t),
 but the independent variable is arbitrary, so it works
 likewise in space

#### 10.2 itransform

inverse of the short time fourier transform

10.3 stft\_

static wrapper for STFT

#### 10.4 stftmat

transformation matrix for the short time fourier transform

#### 10.5 transform

short time fourier transform

## 11 fourier

support and analysis functions both for the discrete (fast) fourier
 transform (dft/fft)
and continuous fourier analysis (fourier series)

## 11.1 amplitude\_from\_peak

```
amplitude and standard deviation of the amplitude of a frequency
   component
represented by a peak in the fourier domain
input :
h : peak height
w : peak width at half height

output:
a : amplitude in real space
s : standard deviation of the frequency (!)
```

#### 11.2 dftmtx\_man

```
fourier matrix in matlab style with a limited number of rows,
columns of higher frequencies are omitted

input :
n : number of samples
nr : number of columns

output :
F : fourier matrix
```

# 11.3 example\_fourier\_window

#### 11.4 fft\_derivative

derivative by fourier transform
exponential convergence for periodic functions
results in spurious oscillations for aperiodic functions
input:
x : data, sampled in equal intervals
k : order of the derivative

dx : kth-derivative of x

#### 11.5 fft\_man

fast fourier transform for complex input data
input:
F : data in real space
output :
F : fourier transformation of F

#### 11.6 fftsmooth

input :
f :
sfunc : a smoothing function (for example fir convolution with
 rectangular window)
 returns filtered (mean) value and normalized fir window
nf : window length
nsigma : number of standard deviations for confidnce intervals

smooth the fourier transform and determine upper and lower bound

output :
ff : filtered fourier transform
l : lower bound
u : upper bound

#### 11.7 fix\_fourier

fill gaps (missing data) by means of fourier extrapolation

fix periodic data series with fourier interpolation
longest gap should not exceed 1/2 of the shortest time span of
 interest (1/cutoff frequency)
note: this limit equals the position of first side lobe of the ft
 of a rectangular window with gap length

#### 11.8 fourier\_axis

return axis of frequencies and periods for the discrete fourier
 transform
as computed by fft (matlab-style)
input:

X : sample locations (equal interval)
L : length of samples

n : number of samples

output :

f : frequencies
T : periods

N : frequency id

#### 11.9 fourier\_cesaro\_correction

#### 11.10 fourier\_coefficient\_piecewise\_linear

fourier series coefficients of a piecewise linear function (not coefficient of discrete fourier transform) function can be discontinuous between intervals scales domain length to 2pi

input :

1,r : end points of piecewise linear function

lval, rval : values at end points

L : length of domain

```
n : number of samples/highest frequency
```

output :

a, b : coefficients for frequency components

## 11.11 fourier\_coefficient\_piecewise\_linear\_1

fourier series coefficients of a piecewise linear function (not coefficient of discrete fourier transform) function can be discontinuous between intervals scales domain length to 2pi

input :

 ${\tt X}$  : end points of piecewise linear function

Y : values at end points

output :

ab : coefficients for frequency components

## 11.12 fourier\_coefficient\_ramp3

fourier series coefficient of a ramp

## 11.13 fourier\_coefficient\_ramp\_pulse

fourier series coefficient of a ramp pules

## 11.14 fourier\_coefficient\_ramp\_step

fourier coefficient of a ramp-step

## 11.15 fourier\_coefficient\_square\_pulse

fourier series coefficients of a square pulse

#### 11.16 fourier\_cubic\_interaction\_coefficients

#### 11.17 fourier\_derivative

coefficients of the derivative of a fourier series not of discrete fourier transform (fft)

## 11.18 fourier\_expand

expand values of fourier series

#### 11.19 fourier\_fit

fit a fourier series to a set of sample points that are not spaced
 in
equal intervals

# 11.20 fourier\_interpolate

interpolate samples y sampled at moments (location) t to locations ti

## 11.21 fourier\_matrix

transformation matrix for a continuous fourier series (not for the discrete dft/fft)

#### 11.22 fourier\_matrix2

transformation matrix for a continuous fourier series (not for the discrete dft/fft)

## 11.23 fourier\_matrix3

transformation matrix for the continous fourier transform this is a matrix with (2\*n+1) real columns

#### 11.24 fourier\_matrix\_exp

transformation matrix for a continuous fourier series (not for the discrete dft/fft)

## 11.25 fourier\_multiplicative\_interaction\_coefficients

#### 11.26 fourier\_power

```
powers of a continuous fourier series in sin/cos form
powers of a^p = (ur + u1 sin(ot) + u2 sin(ot+dp))^p
phase of first component assumed 0
frequencies higher than 2-omega ignored in input
frequencies higher than 3-omega not computed
```

#### 11.27 fourier\_power\_exp

## 11.28 fourier\_predict

expand a continous fourier series at times t

## 11.29 fourier\_quadratic\_interaction\_coefficients

## 11.30 fourier\_range

approximate range of a continous Fourier series with 2 components range(y) = max(y) - min(y)

## 11.31 fourier\_regress

fit a continous fourier series to a set of sample points not
 sampled
at equal intervals

## 11.32 fourier\_resampled\_fit

fits coefficients of a continuous fourier transform, but stores them as resampled values  $\,$ 

#### 11.33 fourier\_resampled\_predict

interpolates a continuous fourier series that has been stored as
 values
at their support points

# 11.34 fourier\_signed\_square

#### 11.35 fourier\_transform

```
continuous fourier transformation of y
(not discrete fourier transformation dft/fft)

input:
    b : data sampled at equal intervals
    T : length of data in time or space, i.e. position of last sample if
    position of first sample is 0
    T_max : maximum period to include

output :
    A : fourier matrix
    p : fourier transformation of b
    tt : TODO
```

#### 11.36 hyperbolic\_fourier\_box

#### 11.37 idftmtx\_man

inverse matrix for the discrete fourier transform in matlab style with a limited number of columns, thus ignoring higher frequencies keep 2nc+1 columns (mean and conj-complex pairs of nc frequencies)

#### 11.38 laplace\_2d\_pwlinear

[x0,p,q,r] piecewise linear polynomials at the boundaries

#### 11.39 nanfft

discrete fourier transform of a data series with gaps

#### 11.40 peaks

#### 11.41 roots\_fourier

```
zeros of continuous fourier series series

f = a_0 + sum_j=^n a_i cos(j x) + b_i sin(j x)
```

#### 11.42 spectral\_density

spectral density

#### 11.43 test\_complex\_exp\_product

#### 11.44 test\_fourier\_filter

#### 11.45 test\_idftmtx

# 12 geometry/@Geometry

## 12.1 Geometry

## 12.2 arclength

```
arc length of a two dimensional curve

8th order accurate does not require the segments length to vary smoothly

note: the curve can be considered parametric, e.g. x = x(t), y=y(t) and

and t = t(s), but the error term contains derivatives of t, thus a non smooth t (strongly varying distance between points) requires the scaling as done below
```

## 12.3 arclength\_old

arc length of a two dimensional function

#### 12.4 arclength\_old2

arc length of a two dimensional function

#### 12.5 base\_point

base point (fusspunkt), i.e. point on a line with shortest distance to another point  $% \left( 1\right) =\left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left$ 

# 12.6 base\_point\_limited

base point (Fusspunkt) of a point on a line

#### 12.7 centroid

centroid pf a polygone

## 12.8 cosa\_min\_max

#### 12.9 cross2

cross product in two dimensions

#### 12.10 curvature

curvature of a function in two dimensions

#### 12.11 ddot

sum of squares of cos of inner angles of triangle

#### 12.12 distance

equclidan distance between two points

#### 12.13 distance2

euclidean distance between two points
this function requires a and be of equal dimensions, or the least
 the first pair or second pair to be a scalar

#### 12.14 dot

dot product

# 12.15 edge\_length

edge length

# 12.16 enclosed\_angle

angle enclosed between two lines

# 12.17 enclosing\_triangle

smallest enclosing equilateral triangle with bottom site paralle to  $\ensuremath{\mathtt{X}}$  axis

## 12.18 hexagon

coordinates of a hexagon, scaled and rotated

# 12.19 inPolygon

flag points contained in a polygon much faster than matlab internal function

# 12.20 inTetra

flag points contained in tetrahedron

#### 12.21 in Tetra 2

flag points contained in tetrahedron

# 12.22 inTriangle

flag points contained in triangle
function [flag, c] = inTriangle(P1,P2,P3,P0)

#### 12.23 intersect

intersect between two lines

## 12.24 lineintersect

intersect of two lines

#### 12.25 lineintersect1

intersect of two lines

## 12.26 minimum\_distance\_lines

minimum distance of two lines in three dimensions

# 12.27 mittenpunkt

mittenpunkt of a triangle

## 12.28 nagelpoint

nagelpoint of a triangle

#### 12.29 onLine

# 12.30 orthocentre

orthocentre of triangle

# 12.31 plumb\_line

## 12.32 poly\_area

area of a polygon
function A = poly\_area(x,y)

## 12.33 poly\_edges

edges of a polygon

## 12.34 poly\_set

associate point at arbitary location with a polygon it is contained in and assign the value of the polygon to it

## 12.35 poly\_width

width of polygon width holes by surface normals holes / islands separated with NaN order of points of outer boundary must be cw order of points of holes must be ccw note that this function does not give the true width for expanding sections use voronoi polygons for this

## 12.36 polyxpoly

intersections of two polygons

# 12.37 project\_to\_curve

closest point on a curve with respect to a point at distance to the  $\ensuremath{\mathtt{curve}}$ 

# 12.38 quad\_isconvex

#### 12.39 random\_disk

draw random points on the unit disk

# 12.40 random\_simplex

random point inside of a triangle

# 12.41 sphere\_volume

volume of a sphere

#### 12.42 tetra\_volume

volume of a tetrahedron

# 12.43 tobarycentric

cartesian to barycentric coordinates

# 12.44 tobarycentric1

cartesian to barycentric coordinates

# 12.45 tobarycentric2

cartesian to barycentric coordinates

# 12.46 tobarycentric3

cartesian to barycentric coordinates

# 12.47 tri\_angle

cos of angles of a triangle

#### 12.48 tri\_area

angle of a triangle

#### 12.49 tri\_centroid

centroid of a triangle

# 12.50 tri\_distance\_opposit\_midpoint

distance between corner of a triangle and its opposing mid-point

# 12.51 tri\_edge\_length

edge length of a triangle

# 12.52 tri\_edge\_midpoint

mid point of a triangle

## 12.53 tri\_excircle

excircle of a triangle

# 12.54 tri\_height

height of a triangle

## 12.55 tri\_incircle

incircle of a triangle

## 12.56 tri\_isacute

flag acute triangles

## 12.57 tri\_isobtuse

flag obntuse triangles

# 12.58 tri\_semiperimeter

semiperimeter of a triangle

# 12.59 tri\_side\_length

edge lenght of triangle

# 13 geometry

## 13.1 Polygon

```
Simple 2D polygon class

Polygon properties:
    x - x coordinates of polygon
    y - y coordinates of polygon
    nnodes - number of nodes in the polygon

Polygon methods:
    in - checks whether given points lie inside, on the edge, or outside of the polygon
    area - returns the area of the polygon
    centerline - computes the centerline of the river
    iscw - check whether polygon is clockwise
    reverse - reverse the order of the polygon
```

## 13.2 bounding\_box

bounding box of X

## 13.3 curvature\_1d

curvature of a sampled parametric curve in two dimensions

#### 13.4 cvt

centroidal voronoi tesselation

## 13.5 deg\_to\_frac

degree, minutes and seconds to fractions

#### 13.6 ellipse

n-points on an ellipse

# 13.7 ellipseX

 ${\tt x\text{-}coordinates}$  of  ${\tt y\text{-}coordinates}$  of an ellipse

# 13.8 ellipseY

## 13.9 first\_intersect

get first intersection between lines in  ${\tt A}$  and  ${\tt B}$ 

# 13.10 golden\_ratio

golden ratio

# 13.11 hypot3

hypothenuse in 3D

# 13.12 meanangle

weighted mean of angles

# 13.13 meanangle2

mean angle

# 13.14 meanangle3

mean angle

## 13.15 meanangle4

mean angle

## 13.16 medianangle

```
median angle angle, that has the smallest squared distance to all others
```

# 13.17 medianangle2

```
median angle
input
alpha : x*m, [rad] angle

ouput
ma : 1*m, [rad] median angle
sa : 1*m, [rad] standard error of median angle for uncorrelated error
```

## 13.18 pilim

```
limit to +- pi
```

## 13.19 streamline\_radius\_of\_curvature

```
streamline radius of curvature simplifies when rotatate to streamwise coordinates to R = 1/dv/ds * u
```

# 14 histogram/@Histogram

#### 14.1 2x

14.3	bimodes
14.4	$\operatorname{cdf}$
14.5	cdfS
14.6	chi2test
14.7	cmoment
14.8	cmomentS
14.9	entropy
14.10	${ m entropyS}$

14.11 iquantile

14.2 Histogram

14.12 kstest

14.13 kurtosis

14.14 kurtosisS

14.15 mean

14.16 meanS

14.17 median

14.18 medianS

14.19 mode

 $14.20 \mod S$ 

14.21 moment

- 14.22 momentS
- 14.23 pdf
- 14.24 quantile
- 14.25 quantileS
- 14.26 setup
- 14.27 skewness
- 14.28 skewnessS
- 14.29 stairs
- 14.30 stairsS
- 14.31 std

 $14.32 \quad stdS$ 

14.33 var

 $14.34 \quad varS$ 

15 histogram

15.1 hist\_man

15.2 histadapt

15.3 histconst

 $15.4 \quad pdf_{-}poly$ 

15.5 plotcdf

15.6 test\_histogram

- 16 linear-algebra
- 16.1 averaging\_matrix\_2
- 16.2 colnorm

norms of columns

16.3 condest\_

estimation of the condition number

# 17 linear-algebra/coordinate-transformation

# 17.1 barycentric2cartesian

barycentric to cartesian coordinates

## 17.2 barycentric2cartesian3

convert barycentric to cartesian coordinates

## 17.3 cartesian2barycentric

cartesian to barycentric coordinates

# $17.4 \quad cartesian\_to\_unit\_triangle\_basis$

transform coodinates into unit triangle

# 17.5 ellipsoid2geoid

# 17.6 example\_approximate\_utm\_conversion

## 17.7 latlon2utm

transform latitude and longitude to WGS84 UTM

# 17.8 latlon2utm\_simple

# $17.9 \quad lowrance\_mercator\_to\_wgs84$

convert lowrance coordinates to wgs84

based on spreadsheet by D Whitney King and Patty B at Lowrance

#### 17.10 nmea2utm

convert nmea messages to utm coordinates

## $17.11 \quad sn2xy$

convert sn to xy coordinates

# $17.12 \quad unit\_triangle\_to\_cartesian$

transform coordinates in unit triangle to cartesian coordinates

## 17.13 utm2latlon

convert wgs84 utm to latitute and longitude

## 17.14 xy2nt

project all points onto the cross section and assign them  $\ensuremath{\text{nz-}}$  coordinates

transform coordinate into N-T reference rotate coordinate, so that cross section goes along x-axis then x and y are n and t respectively scaled by width N and T coordinates  $\begin{array}{c} \text{ To section Boundary Support} \\ \text{ To section Boundary Support$ 

## 17.15 xy2sn

convert cartesian to streamwise coordiantes

## $17.16 \text{ xy}2\text{sn_java}$

use java port for speed up

## 17.17 xy2sn\_old

transform points from cartesian into streamwise coordinates

 $\ensuremath{\mathsf{NOTE}}$  : prefer the java version, this has some problems with round off

# 18 linear-algebra

#### $18.1 \det 2x2$

2x2 matrix inverse of 2x2 matrices stacked along dim 3

#### $18.2 \det 3x3$

determinant of stacked 3x3 matrices

# 18.3 det4x4 determinant of stacked 4x4 matrices 18.4 diag2x2 diagonal of stacked 2x2 matrices

 $18.5 \quad eig2x2$ 

eigenvalues of stacked 2x2 matrices

- 19 linear-algebra/eigenvalue
- 19.1 eig\_bisection
- 19.2 eig\_inverse
- 19.3 eig\_inverse\_iteration
- 19.4 eig\_power\_iteration
- ${\bf 20}\quad {\bf linear-algebra/eigenvalue/jacobi-davids on}$
- 20.1 afun\_jdm

- 20.2 davidson
- 20.3 jacobi\_davidson
- 20.4 jacobi\_davidson\_qr
- 20.5 jacobi\_davidson\_qz
- 20.6 jacobi\_davidson\_simple

#### 20.7 jdqr

```
% Read/set parameters
% Initiate global variables
% Return if eigenvalueproblem is trivial
% Initialize V, W:
  V,W orthonormal, A*V=W*R+Qschur*E, R upper triangular
% The JD loop (Standard)
   V orthogonal, V orthogonal to Qschur
%
   V*V=eye(j), Qschur'*V=0,
%
   W=A*V, M=V,*W
%
\mbox{\ensuremath{\mbox{\%}}} Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

#### 

```
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   Both V and W orthonormal and orthogonal w.r.t. Qschur
%
   V*V=eye(j), Qschur'*V=0, W'*W=eye(j), Qschur'*W=0
%
   (A*V-tau*V)=W*R+Qschur*E, E=Qschur'*(A*V-tau*V), M=W'*V
%
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
\% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
  V W AV.
  Both V and W orthonormal and orthogonal w.r.t. Qschur, AV=A*V-
%
  tau*V
   V*V=eye(j), W'*W=eye(j), Qschur'*V=0, Qschur'*W=0,
%
   (I-Qschur*Qschur')*AV=W*R, M=W'*V; R=W'*AV;
%
\% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

```
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   W orthonormal, V and W orthogonal to Qschur,
   W'*W=eye(j), Qschur'*V=0, Qschur'*W=0
%
   W=(A*V-tau*V)-Qschur*E, E=Qschur'*(A*V-tau*V),
%
   M=W'*V
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
W=V*Q; V=V(:,1:j)/R; E=E/R; R=eye(j); M=Q(1:j,:)'/R;
W=V*H; V(:,j+1)=[]; R=R'*R; M=H(1:j,:)';
%====== ARNOLDI (for initializing spaces)
  _____
%====== END ARNOLDI
  _____
% not accurate enough M=Rw'\(M/Rv);
%====== COMPUTE SORTED JORDAN FORM
  % compute vectors and matrices for skew projection
% solve preconditioned system
% 0 step of bicgstab eq. 1 step of bicgstab
% Then x is a multiple of b
% HIST=[0,1];
explicit preconditioning
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
implicit preconditioning
% collect the updates for x in 1-space
```

```
% but, do the orth to Q implicitly
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
% Do the orth to Q explicitly
\% In exact arithmetic not needed, but
% appears to be more stable.
% plot(HIST(:,1),log10(HIST(:,2)+eps),'*'), drawnow, pause
\% 0 step of gmres eq. 1 step of gmres
% Then x is a multiple of b
% O step of gmres eq. 1 step of gmres
% Then x is a multiple of b
HIST=1;
% Lucky break-down
HIST=[HIST; (gamma~=0)/sqrt(rho)];
% Lucky break-down
% solve in least square sense
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow,% pause
r=r/rho; rho=1;
% HIST=rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow,% pause
% HIST = rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow, pause
% HIST = rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow, pause
%----- compute schur form -----
A*Q=Q*S, Q'*Q=eye(size(A));
\% transform real schur form to complex schur form
\%----- find order eigenvalues -----
%----- reorder schur form ------
%----- compute qz form ------
%----- sort eigenvalues ------
%----- sort qz form -----
% i>j, move ith eigenvalue to position j
% determine dimension
% defaults
%% 'v'
```

#### 20.8 jdqr\_sleijpen

```
% Read/set parameters
% Initiate global variables
% Return if eigenvalueproblem is trivial
% Initialize V, W:
  V,W orthonormal, A*V=W*R+Qschur*E, R upper triangular
% The JD loop (Standard)
   V orthogonal, V orthogonal to Qschur
   V*V=eye(j), Qschur'*V=0,
%
   W=A*V, M=V, *W
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   Both V and W orthonormal and orthogonal w.r.t. Qschur
   V*V=eye(j), Qschur'*V=0, W'*W=eye(j), Qschur'*W=0
%
   (A*V-tau*V)=W*R+Qschur*E, E=Qschur'*(A*V-tau*V), M=W'*V
%
\mbox{\ensuremath{\mbox{\%}}} Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

```
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   V W AV.
%
   Both V and W orthonormal and orthogonal w.r.t. Qschur, AV=A*V-
%
   V*V=eye(j), W'*W=eye(j), Qschur'*V=0, Qschur'*W=0,
%
   (I-Qschur*Qschur')*AV=W*R, M=W'*V; R=W'*AV;
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
\% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   W orthonormal, V and W orthogonal to Qschur,
%
   W'*W=eye(j), Qschur'*V=0, Qschur'*W=0
   W=(A*V-tau*V)-Qschur*E, E=Qschur'*(A*V-tau*V),
%
   M=W,*V
%
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
\% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

```
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
W=V*Q; V=V(:,1:j)/R; E=E/R; R=eye(j); M=Q(1:j,:)'/R;
W=V*H; V(:,j+1)=[];R=R'*R; M=H(1:j,:)';
%====== ARNOLDI (for initializing spaces)
   %===== END ARNOLDI
   % not accurate enough M=Rw'\(M/Rv);
%====== COMPUTE SORTED JORDAN FORM
   _____
\% compute vectors and matrices for skew projection
% solve preconditioned system
% 0 step of bicgstab eq. 1 step of bicgstab
% Then x is a multiple of b
% HIST=[0,1];
explicit preconditioning
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
implicit preconditioning
% collect the updates for x in 1-space
% but, do the orth to Q implicitly
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
\% Do the orth to Q explicitly
% In exact arithmetic not needed, but
% appears to be more stable.
% plot(HIST(:,1),log10(HIST(:,2)+eps),'*'), drawnow, pause
\% 0 step of gmres eq. 1 step of gmres
% Then x is a multiple of b
%-----
% O step of gmres eq. 1 step of gmres
% Then x is a multiple of b
HIST=1;
% Lucky break-down
HIST=[HIST; (gamma~=0)/sqrt(rho)];
% Lucky break-down
% solve in least square sense
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow,% pause
r=r/rho; rho=1;
% HIST=rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
```

```
plot(J,HIST(:,1),'*'); drawnow,% pause
% HIST = rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow, pause
% HIST = rho;
% HIST=[HIST;rho];
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1];
plot(J,HIST(:,1),'*'); drawnow, pause
%----- compute schur form -----
A*Q=Q*S, Q'*Q=eye(size(A));
% transform real schur form to complex schur form
%----- find order eigenvalues ------
%----- reorder schur form ------
%----- compute qz form ------
%----- sort eigenvalues ------
%----- sort qz form -----
% i>j, move ith eigenvalue to position j
% determine dimension
% defaults
%% 'v'
```

## $20.9 \quad jdqr\_vorst$

```
% Read/set parameters
% Initiate global variables
% Return if eigenvalueproblem is trivial
% Initialize V, W:
 V,W orthonormal, A*V=W*R+Qschur*E, R upper triangular
% The JD loop (Standard)
   V orthogonal, V orthogonal to Qschur
%
   V*V=eye(j), Qschur'*V=0,
%
   W=A*V, M=V*W
%
\mbox{\ensuremath{\mbox{\%}}} Compute approximate eigenpair and residual
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

```
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   Both V and W orthonormal and orthogonal w.r.t. Qschur
   V*V=eye(j), Qschur'*V=0, W'*W=eye(j), Qschur'*W=0
%
   (A*V-tau*V)=W*R+Qschur*E, E=Qschur'*(A*V-tau*V), M=W'*V
% Compute approximate eigenpair and residual
%
%
%
%
% Check for convergence
% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
  V W AV.
%
  Both V and W orthonormal and orthogonal w.r.t. Qschur, AV=A*V-
%
   V*V=eye(j), W'*W=eye(j), Qschur'*V=0, Qschur'*W=0,
   (I-Qschur*Qschur')*AV=W*R, M=W'*V; R=W'*AV;
%
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
\% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
```

```
% Expand preconditioned Schur matrix PinvQ
\% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
% The JD loop (Harmonic Ritz values)
   W orthonormal, V and W orthogonal to Qschur,
   W'*W=eye(j), Qschur'*V=0, Qschur'*W=0
%
   W=(A*V-tau*V)-Qschur*E, E=Qschur'*(A*V-tau*V),
   M=W'*V
% Compute approximate eigenpair and residual
%
%
%
% Check for convergence
\% Expand the partial Schur form
Rschur=[[Rschur;zeros(1,k)],Qschur'*MV(u)]; k=k+1;
% Expand preconditioned Schur matrix PinvQ
% Check for shrinking the search subspace
% Solve correction equation
% Expand the subspaces of the interaction matrix
W=V*Q; V=V(:,1:j)/R; E=E/R; R=eye(j); M=Q(1:j,:)'/R;
W=V*H; V(:,j+1)=[];R=R'*R; M=H(1:j,:)';
%====== ARNOLDI (for initializing spaces)
   %====== END ARNOLDI
   _____
% not accurate enough M=Rw'\(M/Rv);
%====== COMPUTE SORTED JORDAN FORM
   _____
% accepted separation between eigenvalues:
% no preconditioning
% solve left preconditioned system
% compute vectors and matrices for skew projection
% precondion and project r
\% solve preconditioned system
% no preconditioning
% solve two-sided expl. precond. system
% compute vectors and matrices for skew projection
% precondion and project r
% solve preconditioned system
% "unprecondition" solution
%%%% u(:,j+1)=Atilde*u(:,j)
```

### 20.10 jdqz

```
% Read/set parameters
% Return if eigenvalueproblem is trivial
\mbox{\ensuremath{\%}} Initialize target, test space and interaction matrices
% V=RepGS(Qschur,V); [AV,BV]=MV(V); %%% more stability??
% W=RepGS(Zschur,eval(testspace)); %%% dangerous if sigma~lambda
% Solve the preconditioned correction equation
% Expand the subspaces and the interaction matrices
% Check for stagnation
% Solve projected eigenproblem
% Compute approximate eigenpair and residual
%=== an alternative, but less stable way of computing z =====
% display history
% save history
% check convergence
% EXPAND Schur form
% Expand preconditioned Schur matrix MinvZ=M\Zschur
\% check for conjugate pair
% To detect whether another eigenpair is accurate enough
% restart if \dim(V) > \max
% Initialize target, test space and interaction matrices
% additional stabilisation. May not be needed
% V=RepGS(Zschur,V); [AV,BV]=MV(V);
% end add. stab.
% Solve the preconditioned correction equation
% expand the subspaces and the interaction matrices
% Check for stagnation
% compute approximate eigenpair
\% Compute approximate eigenpair and residual
% display history
% save history
% check convergence
% expand Schur form
```

```
% ZastQ=Z'*Q0
% the final Qschur
% check for conjugate pair
% t perp Zschur, t in span(Q0,imag(q))
% To detect whether another eigenpair is accurate enough
% restart if dim(V)> jmax
%===== END JDQZ
%====== PREPROCESSING
 ______
%====== ARNOLDI (for initial spaces)
 _____
%% then precond=I and target = 0: apply Arnoldi with A
%===== END ARNOLDI
 _____
%====== POSTPROCESSING
%-----
%====== SORT QZ DECOMPOSITION INTERACTION MATRICES
 ==============
%====== COMPUTE SORTED JORDAN FORM
 _____
%====== END JORDAN FORM
 ______
%====== OUTPUT
 ______
%====== UPDATE PRECONDITIONED SCHUR VECTORS
 %====== SOLVE CORRECTION EQUATION
 _____
% solve preconditioned system
%-----
```

```
%====== LINEAR SOLVERS
   % [At,Bt]=MV(x); At=theta(2)*At-theta(1)*Bt;
% xtol=norm(r-At+Z*(Z'*At))/norm(r);
%===== Iterative methods
% 0 step of bicgstab eq. 1 step of bicgstab
\% Then x is a multiple of b
% HIST=[0,1];
explicit preconditioning
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
implicit preconditioning
% collect the updates for x in 1-space
% but, do the orth to Z implicitly
% compute norm in 1-space
% HIST=[HIST; [nmv,rnrm/snrm]];
% sufficient accuracy. No need to update r,u
% Do the orth to Z explicitly
% In exact arithmetic not needed, but
% appears to be more stable.
% plot(HIST(:,1),log10(HIST(:,2)+eps),'*'), drawnow
% O step of gmres eq. 1 step of gmres
% Then x is a multiple of b
% O step of gmres eq. 1 step of gmres
% Then x is a multiple of b
HIST=1;
% Lucky break-down
HIST=[HIST; (gamma~=0)/sqrt(rho)];
% Lucky break-down
% solve in least square sense
HIST=log10(HIST+eps); J=[0:size(HIST,1)-1]';
plot(J,HIST(:,1),'*'); drawnow
%===== END SOLVE CORRECTION EQUATION
   _____
%====== BASIC OPERATIONS
y(1:5,1), pause
%====== COMPUTE r AND z
   ______
```

```
% E*u=Q*sigma, sigma(1,1)>sigma(2,2)
\%====== END computation r and z
 _____
\%======= Orthogonalisation
 _____
%===== END Orthogonalisation
 %====== Sorts Schur form
 _____
kappa=max(norm(A,inf)/max(norm(B,inf),1.e-12),1);
 kappa=2^(round(log2(kappa)));
\%----- compute the qz factorization ------
\%----- scale the eigenvalues -----
\%----- sort the eigenvalues -----
%----- swap the qz form ------
% repeat SwapQZ if angle is too small
\% i>j, move ith eigenvalue to position j
% compute q s.t. C*q=(t(i,1)*S-s(i,1)*T)*q=0
C*P=Q*R
check whether last but one diag. elt r nonzero
C*q
% end computation q
\mbox{\%======} END sort QZ decomposition interaction matrices
 =========
%====== INITIALIZATION
    -----
% defaults
          %%%% search for 'xx' in fieldnames
%% 'ma'
%% 'sch'
%% 'to'
%% 'di'
```

```
% jmin=nselect+p0 %%%% 'jmi'
% jmax=jmin+p1 %%%% 'jma'
%% 'te'
%% 'pai'
%% 'av'
%% 'tr'
%% 'fix'
%% 'ns'
%% 'ch'
%% 'lso'
%% 'ls_m'
%% 'ls_t'
%% 'ls_e'
%% 'ty'
%% '1_'
%% 'u_'
%% 'p_'
%% 'sca'
%% 'v0'
initiation
'standard'
'harmonic'
'searchspace'
% or Operator_Form=3 or Operator_Form=5???
%====== DISPLAY FUNCTIONS
```

## $20.11 \quad mfunc_{jdm}$

#### 20.12 mgs

#### $20.13 \quad minres_{-}$

## $20.14 \quad mv_{jacobi\_davidson}$

# 21 linear-algebra

#### 21.1 first

## ${\bf 21.2} \quad {\bf gershgorin\_circle}$

range of eigenvalues determined by the gershgorin circle theorem

#### 21.3 haussdorff

```
haussdorf dimension box counting: count cectangles passed through by line (covered by polygon)
```

```
Koch snow flake 3:4 \rightarrow 1.2619
Kantor set 2:3, (4:9) \rightarrow 0.6309
quadrat 4:2, 9:3, 16:4 \rightarrow 2
```

## 21.4 ieig2x2

reconstruct matrix from eigenvalue decomposition

#### 21.5 inv2x2

2x2 inverse of stacked matrices

21.6 inv3x3
21.7 inv4x4
inverse of stacked 4x4 matrices
22  linear-algebra/lanczos
22.1 arnoldi
$22.2  arnoldi_new$
22.3 eigs_lanczos_man
22.4 lanczos
$22.5$ lanczos $_{-}$
$22.6$ lanczos_biorthogonal

 ${\bf 22.7} \quad lanczos\_biorthogonal\_improved$ 

- 22.8 lanczos\_ghep
- 22.9 mv\_lanczos
- 22.10 reorthogonalise
- 22.11 test\_lanczos
- ${\bf 23}\quad {\bf linear-algebra/linear-systems}$
- 23.1 gmres\_man

break on convergence

23.2 minres\_recycle

- 24 linear-algebra
- 24.1 lpmean

mean of pth-power of a

24.2 lpnorm

norm of 1th-power of a

#### 24.3 matvec3

matrix-vector product of stacked matrices and vectors

## 24.4 max2d

maximum value and i-j index for matrix

## 24.5 mpoweri

approximation of A^p, where p is not integer by quadtratic interpolation

#### $24.6 \quad \text{mtimes} 2x2$

#### 24.7 mtimes3x3

product of stacked 3x3 matrices

#### 24.8 nannorm

norm of a vector, skips nan-values

## 24.9 nanshift

shift vector, but set out of range values to NaN

#### 24.10 nl

number rows (lines) of a matrix analogue to unix nl command

#### 24.11 normalise

```
normalise a vector or the columns of a matrix
note that the columns are independently normalised, and hence not
   necessarily
orthogonal to each other use the gram schmidt algorithm for this (
   qr or orth)
```

## 24.12 normalize1

```
normalize columns in x to [-1,1]
```

#### 24.13 normrows

#### 24.14 orth2

make matrix A orhogonal to B

#### 24.15 orth\_man

orthogonalize the columns of  ${\tt A}$ 

## 24.16 orthogonalise

make x orthogonal to Y

## 24.17 paddext

```
padd values to vactor
not suitable for noisy data
order = 0 : constant extrapolation (hold)
order = 1 : linear extrapolation
```

## 24.18 paddval1

padd values at end of x

## 24.19 paddval2

padd values to x

# 25 linear-algebra/polynomial

## 25.1 chebychev

chebycheff polynomials

## 25.2 piecewise\_polynomial

evaluate piecewise polynomial

#### 25.3 roots1

roots of linear functions

### 25.4 roots2

roots of quadratic function  $c1 x^2 + c2 x + c3 = 0$ 

## 25.5 roots2poly

### 25.6 roots3

## 25.7 roots4

## 25.8 test\_roots4

#### 25.9 vanderi\_1d

vandermonde matrix of an integral

# 26 linear-algebra

## 26.1 randrot

random rotation matrix

## **26.2** right

get right column by shifting columns to left extrapolate rightmost column  $\,$ 

## 26.3 rot2

rotation matrix from angle

#### 26.4 rot2dir

rotation matrix from direction vector

### 26.5 rot3

26.	6	$\operatorname{rot} \mathbf{R}$
40.		1001

- 26.7 rownorm
- $26.8 \quad simmilarity\_matrix$
- 26.9 spnorm

frobenius norm

26.10 spzeros

allocate a sparze matrix of zeros

- $26.11 \quad test\_roots3$
- 26.12 transform\_minmax
- 26.13 transpose3

transpose stacked 3x3 matrices

26.14 transposeall

# 27 logic

bitwise operations on integers

## 27.1 bitor\_man

bitwise OR of the numbers of the columns of A
input:
 A (positive integer)

- 28 master/plot
- 28.1 attach\_boundary\_value
- ${\bf 28.2 \quad cartesian\_polar}$
- 28.3 img\_vargrid
- $28.4 \quad plot\_basis\_functions$
- 28.5 plot\_convergence
- $28.6 \quad plot\_dof$
- 28.7 plot\_eigenbar

- $28.8 \quad plot\_error\_estimation$
- $28.9 \quad plot\_error\_estimation\_2$
- 28.10 plot\_error\_fem
- $28.11 \quad plot\_fdm\_kernel$
- $28.12 \quad plot\_fdm\_vs\_fem$
- $28.13 \quad plot\_fem\_accuracy$
- $28.14 \quad plot\_function\_and\_grid$
- 28.15 plot\_hat
- 28.16 plot\_hydrogen\_wf
- 28.17 plot\_mesh

- $28.18 \quad plot\_mesh\_2$
- 28.19 plot\_refine
- 28.20 plot\_refine\_3d
- 28.21 plot\_runtime
- 28.22 plot\_spectrum
- 28.23 plot\_wavefunction
- 29 master/ported
- $29.1 \quad assemble\_2d\_dphi\_dphi$
- 29.2 assemble\_2d\_phi\_phi
- $29.3 \quad assemble\_3d\_dphi\_dphi$

- $29.4 \quad assemble\_3d\_phi\_phi$
- $29.5 \quad dV_- 2d_-$
- 29.6 derivative\_2d
- 29.7 derivative\_3d
- 29.8 element\_neighbour\_2d
- $29.9 \quad prefetch\_2d\_$
- $29.10 \quad promote\_2d\_3\_10$
- $29.11 \quad promote\_2d\_3\_15$
- $29.12 \quad promote\_2d\_3\_21$
- $29.13 \quad promote\_2d\_3\_6$

- $29.14 \quad promote\_3d\_4\_10$
- $29.15 \quad promote\_3d\_4\_20$
- $29.16 \quad promote\_3d\_4\_35$
- 29.17 vander\_2d
- 29.18 vander\_3d
- $30 \quad master/sandbox$
- 30.1 adapt
- 30.2 assoc\_laguerre
- 30.3 assoc\_legendre
- 30.4 c23

31	${ m master/sandbox/cg}$
31.1	cg
31.2	$cg\_coef\_to\_poly$
31.3	errmat
31.4	lanczos
31.5	laplacian_2d
R1 6	${ m test\_cg\_eigs}$
<b>J1.</b> 0	1031_08_0183
31.7	${ m test\_lanczos}$
32	master/sandbox
	condition_number_higher_order
·±	condition_mamoor_mgnor_order

 ${\bf 32.2} \quad confinement\_dat$ 

32.3	convergence_2d_3d
32.4	$convergence\_matrix\_powers$
32.5	$\operatorname{cut}$ _out
32.6	${\bf derivative\_2d}$
32.7	${\bf derivative\_3d}$
32.8	dummy
32.9	eig_error
32.10	eigs_fix
32.11	energy_level

32.12 equalise

## 32.13 example\_int64

Basic operations

Matrix multiplication Timing

- $33 \quad master/s and box/fem-matlab$
- 33.1 boundary\_circle
- 33.2 boundary\_rectangle
- 33.3 geometry\_circle\_with\_hole
- 33.4 geometry\_rectangle
- 34 master/sandbox
- 34.1 fem\_2d\_estimate\_error
- 34.2 fem\_assemble\_scratch

34.3	$\mathrm{fem}_{-\mathrm{s}}$
34.4	fourier_h
34.5	grad_2d
34.6	grad_3d
34.7	gradient
34.8	$harmonic\_oscillator$
34.9	$hydrogen\_2d\_analytic$
34.10	$hydrogen\_boxed$

 $34.11 \quad hydrogen\_boxed\_old$ 

34.12 hydrogen\_wave

% Hydrogen atom

34.14	$ichol\_man$
34.15	$known\_eigenvalue$
34.16	kron_man
34.17	laguerre
34.18	laplacian_arbitrary_order_old
34.19	$laplacian\_convergence$
34.20	$laplacian\_cut\_out$
34.21	laplacian_cylindrical
34.22	laplacian_non_uniform_old

 $34.13 \quad hydrogen\_wf$ 

34.23	laplacian_polar
34.24	laplacian_simple
34.25	lderivative_3d
34.26	${ m list}_{ m d}{ m at}$
34.27	matlab-horner
34.28	$mesh\_to\_grid\_2d\_3$
34.29	$mg\_mat$
34.30	mv

 ${\bf 34.32 \quad partial\_derivative\_2d}$ 

34.31 orth2

34.33	$partition\_function$
34.34	$partition\_function\_old$
34.35	poisson
34.36	poisson_fem
34.37	potential
34.38	powerc
34.39	$\operatorname{quick\_newihbour}$
34.40	radial
34.41	radial_convergence

34.42 radial\_wafefunction

34.43 refine\_2d

34.44 refine\_3d

**34.45** relerr

34.46 restore\_cw

34.47 runtime\_bm

34.48 rydberg

34.49 s\_old

34.50 snorm

34.51 spherical\_harmonic

34.52 split\_eig

34.53 sum1
34.54 sum3
35 master/sandbox/summation
35.1 acc
35.2 add
35.3 ape
35.4 mmul_accurately
35.5 sum_kahan

 $35.6 \quad sum\_pairwise$ 

35.7 test\_sum

36	master/sandbox
36.1	$test\_convergence\_ill\_conditioned$
36.2	${ m test\_fem\_1d}$
36.3	${ m test\_fem\_2d}$
36.4	${ m test\_fem\_3d}$
36.5	$test\_increase$
36.6	$test\_lanczos\_shift$

 $36.9 \quad trefethen\_p8\_fdm$ 

 $36.7 \quad test\_ldl$ 

 $36.8 test\_power$ 

### 36.10 wavefunc

## 36.11 xgrid

# 37 number-theory

## 37.1 ceiln

floor to leading n-digits

# 37.2 digitsb

number of digits with respect to specified base

#### 37.3 floorn

floor to n-digits

### 37.4 iseven

true for even numbers in X

### 37.5 multichoosek

all combinations of lenght k from set values with repetitions c.f. nchoosek, combinations without repetition

input :

 ${\bf x}$  : scalar integer or vector of arbitrary numbers

k : length of subsets

output :

if  $\boldsymbol{x}$  scalar : number of combinations if  $\boldsymbol{x}$  vector : the exact combinations

### 37.6 nchoosek\_man

vecotrised binomial coefficient b = N!/K!(N-K)!

# 37.7 pythagorean\_triple

pythagorean triple

### 37.8 roundn

round to n digits

# 38 numerical-methods/differentiation

## 38.1 derivative1

first derivative on variable mesh second order accurate

### 38.2 derivative2

second derivative on a variable mesh

# 39 numerical-methods/finite-difference

### 39.1 cdiff

differences of columns of X
degree = 1 : central first order differences
degreee = 2 : central second order differences

### 39.2 cdiffb

differences of columns of X
degree = 1 : central first order differences
degreee = 2 : central second order differences
TODO use difference matrix function for simplicity

#### 39.3 cmean

single gaussian smoothing step with kernel 1/4\*[1,2,1]

### 39.4 derivative\_matrix\_1\_1d

finite difference matrix of first derivative in one dimensions

### 39.5 derivative\_matrix\_2\_1d

finite derivative matrix of second derivative in one dimension

## 39.6 derivative\_matrix\_2d

finite difference derivative matrix in two dimensions

### 39.7 derivative\_matrix\_curvilinear

derivative matrix on a curvilinear grid

# 39.8 derivative\_matrix\_curvilinear\_2

derivative matrix on a two dimensional curvilinear grid the grid has not necessarily to be orthogonal

# 39.9 difference\_kernel

difference kernels for equispaced grids c.f. Computing the Spectrum of the Confined Hydrogen Atom, Kastner, 2012

#### 39.10 distmat

distance matrix for a 2 dimensional rectangular matrix

## 39.11 gradpde2d

```
objective function gradiend on two dimensional regular grid numeric gradient for non-linear least squares optimisation of a PDE on a rectangular grid x_* = \min(f(x)) f = (v(x) - v(x_*))^2 = f(x) + A dx + O(dx^2) a_ij = df_i/dx_j
```

### 39.12 laplacian

## 39.13 laplacian\_fdm

finite difference matrix of the laplacian  $\ensuremath{\mathsf{BC}}$ 

#### 39.14 left

left element of vector, leftmost column is extrapolated

#### 39.15 lrmean

mean of the left and right element

numerical-methods/finite-difference/master**40** 40.1  $fdm\_adaptive\_grid$  $fdm_adaptive_refinement_old$ 40.3 fdm\_assemble\_d1\_2d  $40.4 \quad fdm\_assemble\_d2\_2d$ 40.5  $fdm_{-}confinement$ 40.6 fdm\_d\_vargrid 40.7  $fdm_h_unstructured$ fdm\_hydrogen\_vargrid 40.8 40.9fdm\_mark\_unstructured\_2d

40.10	$fdm_{-}plot$	
40.11	$fdm\_plot\_series$	
40.12	$fdm_refine_2d$	
40.13	$fdm_refine_3d$	
40.14	$fdm\_refine\_unstructured\_2d$	
40.15	$fdm\_schroedinger\_2d$	
40.16	$fdm\_schroedinger\_3d$	
40.17	relocate	
<b>41</b> r	numerical-methods/finite-difference	
41.1 mid		

mid point between neighbouring vector elements

# 41.2 pwmid

segment end point to segment mid point transformation for regular 1  $\,$  d grids  $\,$ 

# 41.3 ratio

ratio of two subsequent values

# 41.4 steplength

step length of a vector if it were equispaced

# 41.5 swapoddeven

swap odd and even elements in a vector

## 41.6 test\_derivative\_matrix\_2d

## 41.7 test\_derivative\_matrix\_curvilinear

### 41.8 test\_difference\_kernel

# ${\bf 42} \quad numerical - methods/finite-element$

# 42.1 Mesh\_2d\_java

- $42.2 \quad Tree\_2d\_java$
- 42.3 assemble\_1d\_dphi\_dphi
- 42.4 assemble\_1d\_phi\_phi
- 42.5 assemble\_2d\_dphi\_dphi\_java
- 42.6 assemble\_2d\_phi\_phi\_java
- $42.7 \quad assemble\_3d\_dphi\_dphi\_java$
- $42.8 \quad assemble\_3d\_phi\_phi\_java$
- 42.9 boundary\_1d
- 42.10 boundary\_2d
- 42.11 boundary\_3d

- 42.12 check\_area\_2d
- 42.13 circmesh
- 42.14 cropradius
- $42.15 \quad display\_2d$
- 42.16 display\_3d
- **42.17** distort
- $42.18 \quad err_2d$
- 42.19 estimate\_err\_2d\_3
- 42.20 example\_1d
- 42.21 example\_2d

- 42.22 explode
- 42.23 fem<sub>2</sub>d
- 42.24 fem\_2d\_heuristic\_mesh
- $42.25 \quad fem\_get\_2d\_radial$
- 42.26 fem\_interpolation
- $42.27 \quad fem\_plot\_1d$
- $42.28 \quad fem\_plot\_1d\_series$
- 42.29 fem\_plot\_2d
- 42.30 fem\_plot\_2d\_series
- 42.31 fem\_plot\_3d

- $42.32 \quad fem\_plot\_3d\_series$
- ${\bf 42.33 \quad fem\_plot\_confine\_series}$
- 42.34 fem\_radial

adaptive grid constant grid

- $42.35 \quad flip\_2d$
- $42.36 \quad get\_mesh\_arrays$
- 42.37 hashkey
- $43 \quad numerical-methods/finite-element/int$
- $43.1 \quad int\_1d\_gauss$
- $43.2 \quad int\_1d\_gauss\_1$
- $43.3 \quad int\_1d\_gauss\_2$

- $43.4 \quad int\_1d\_gauss\_3$
- $43.5 \quad int\_1d\_gauss\_4$
- $43.6 \quad int\_1d\_gauss\_5$
- $43.7 \quad int\_1d\_gauss\_6$
- $43.8 \quad int\_1d\_gauss\_lobatto$
- $43.9 \quad int\_1d\_nc\_2$
- $43.10 \quad int\_1d\_nc\_3$
- $43.11 \quad int\_1d\_nc\_4$
- $43.12 \quad int\_1d\_nc\_5$
- 43.13 int\_1d\_nc\_6

- $43.14 \quad int\_1d\_nc\_7$
- 43.15 int\_1d\_nc\_7\_hardy
- 43.16 int\_2d\_gauss\_1
- $43.17 \quad int\_2d\_gauss\_12$
- 43.18 int\_2d\_gauss\_13
- $43.19 \quad int\_2d\_gauss\_16$
- $43.20 \quad int\_2d\_gauss\_25$
- $43.21 \quad int\_2d\_gauss\_3$
- $43.22 \quad int\_2d\_gauss\_33$
- $43.23 \quad int\_2d\_gauss\_6$

- $43.24 \quad int\_2d\_gauss\_7$
- $43.25 \quad int\_2d\_gauss\_9$
- $43.26 \quad int\_2d\_nc\_10$
- 43.27 int\_2d\_nc\_15
- 43.28 int\_2d\_nc\_21
- $43.29 \quad int\_2d\_nc\_3$
- 43.30 int\_2d\_nc\_6
- $43.31 \quad int_3d_gauss_1$
- $43.32 \quad int\_3d\_gauss\_11$
- $43.33 \quad int\_3d\_gauss\_14$

- $43.34 \quad int\_3d\_gauss\_15$
- $43.35 \quad int\_3d\_gauss\_24$
- $43.36 \quad int\_3d\_gauss\_4$
- $43.37 \quad int\_3d\_gauss\_45$
- $43.38 \quad int\_3d\_gauss\_5$
- $43.39 \quad int\_3d\_nc\_11$
- 43.40 int\_3d\_nc\_4
- $43.41 \quad int\_3d\_nc\_6$
- $43.42 \quad int\_3d\_nc\_8$

44	numerical - methods/finite-element
44.1	$interpolation\_matrix$
44.2	mark
44.3	$ m mark_1d$
44.4	$mesh\_1d\_uniform$
44.5	${ m mesh\_3d\_uniform}$
44.6	$\operatorname{mesh\_interpolate}$
44.7	$ m neighbour\_1d$
44.8	old

44.9 pdeeig\_1d

- 44.10 pdeeig\_2d
- 44.11 pdeeig\_3d
- 44.12 polynomial\_derivative\_1d
- 44.13 potential\_const
- 44.14 potential\_coulomb
- $44.15 \quad potential\_harmonic\_oscillator$
- 44.16 project\_circle
- 44.17 project\_rectangle
- $44.18 \quad promote\_1d\_2\_3$
- 44.19 promote\_ $1d_2_4$

- $44.20 \quad promote\_1d\_2\_5$
- $44.21 \quad promote\_1d\_2\_6$
- 44.22 quadrilaterate
- $44.23 \quad recalculate\_regularity\_2d$
- 44.24 refine\_1d
- 44.25 refine\_2d\_21
- 44.26 refine\_2d\_structural
- 44.27 regularity\_1d
- $44.28 \quad regularity\_2d$

```
44.29 \quad regularity\_3d
       T = [1 \ 2 \ 3 \ 4];
44.30 \quad relocate\_2d
44.31 test_circmesh
44.32 test_hermite
44.33 tri_assign_points
44.34 triangulation_uniform
44.35 vander_1d
van der Monde matrix
```

44.37 vanderi\_1d

44.36 vanderd<sub>-</sub>1d

# 45 numerical-methods/finite-volume/@Advection

### 45.1 Advection

FVM treatment of the Advection equation

## 45.2 dot\_advection

advection equation

# 46 numerical-methods/finite-volume/@Burgers

### 46.1 burgers\_split

```
viscous Burgers' equation, mixed analytic and numerical derivative in frequency space by splitting sheme u_t = -(0.5*u^2)_x + c*u_xx
```

## 46.2 dot\_burgers\_fdm

```
viscous burgers' equation

u_t = -d/dx (1/2*u^2) + c d^2/dx^2 u_xx
```

### 46.3 dot\_burgers\_fft

```
viscous Burgers' equation in frequency space u_t + (0.5*u^2)_x = c*u_xx
```

# 47 numerical-methods/finite-volume/@Finite\_Volume

# 47.1 Finite\_Volume

```
finite volume method for partial differential equations 1+1
    dimensions
(time and space)
```

# 47.2 apply\_bc

apply boundary conditions

#### 47.3 solve

### 47.4 step\_split\_strang

step in time, treat inhomogeneous part by Strang splitting this scheme is not suitable for stationary solutions, for example steady shallow water flow

### 47.5 step\_unsplit

step in time, without splitting the inhomogeneous term

# 48 numerical-methods/finite-volume/@Flux\_Limiter

### 48.1 Flux\_Limiter

class of flux limiters

## 48.2 beam\_warming

beam warming sheme
low resolution
note: works only if sign of eigenvalues point into the same
direction according to RL

### 48.3 fromm

fromme limiter
low res

## $48.4 lax_wendroff$

lax wendroff scheme second order accurate, but no tvd this is effectively not a limiter eq. 6.39 in randall, leveque

### 48.5 minmod

min-mod schock limiter

## 48.6 monotized\_central

monotonized central flux limiter

### 48.7 muscl

muscl flux limiter

# 48.8 superbee

superbee limiter

# 48.9 upwind

godunov scheme
godunov, first order accurate

#### 48.10 vanLeer

van Leer limiter

# 49 numerical-methods/finite-volume/@KDV

## $49.1 \quad dot_kdv_fdm$

```
korteweg de vries equation u_t + (0.5*u^2)_x = c*u_xxx
```

#### 49.2 dot\_kdv\_fft

```
korteweg de vries equation compute derivatives in frequency space u_t + (0.5*u^2)_x = c*u_xxx
```

# $49.3 kdv\_split$

korteweg de vries equation in frequency space, derivative treated by splitting scheme

# $50 \quad numerical-methods/finite-volume/@Reconstruct\_Average\_E$

### 50.1 Reconstruct\_Average\_Evolve

## 50.2 advect\_highres

single time step for the reconstruct evolve algorithm

### 50.3 advect\_lowress

single time step
low resolution

# 51 numerical-methods/finite-volume

### 51.1 Godunov

Godunov, upwind method for systems of pdes

### 51.2 Lax\_Friedrich

Lax-Friedrich-Method
for hyperbolic conservation laws
err = O(dt) + O(dx)
|a dt/dx| < 1</pre>

#### 51.3 Measure

## 51.4 Roe

non linear roe solver for the SWE (randall, leveque 15.3.1)

The roe solver guarantess:

- $\mbox{A}$  is diagonalisable with real eigenvalues (15.12)
- can be determined by a closed formula
- is an efficient replacement for true Rieman solver

#### 51.5 fv\_swe

wrapper for solving SWE

## 51.6 staggered\_euler

forward euler method with staggered grid

## 51.7 staggered\_grid

staggered grid approximation to the SWE

# 52 numerical-methods

# 52.1 grid2quad

extract rectangular elements of a structured grid in form of an unstructured quad-mesh format  $\,$ 

# 53 numerical-methods/integration

#### 53.1 cumintL

cumulative integral from left to right

### 53.2 cumintR

cumulative integral from right to left

# 53.3 int\_trapezoidal

integrate y along x with the trapezoidal rule

# 54 numerical-methods/interpolation/@Kriging

## 54.1 Kriging

class for Kriging interpolation

#### 54.2 estimate\_semivariance

estimate the parameter of the semivariance model for Kriging interpolation  $% \left( 1\right) =\left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left( 1\right) +\left( 1\right) \left( 1$ 

% set up the regression matrix and solve for parameters

### 54.3 interpolate\_

interpolate with Krieging method

this function may interpolate several quantities per coordinate, using the same variogram, if the semivariance of the quantities differs,

the user may prefer to estimate the semivariance and interpolate each quantity individually

Xs : source point coordinates
Vs : value at source points
Xt : targe point coordinates
Vt : value at target points

E2t : squared interpolation error at target points

# $55 \quad numerical-methods/interpolation/@RegularizedInterpolator 1$

# 55.1 RegularizedInterpolator1

class for regularized interpolation (Thikonov) on a 1D mesh

### 55.2 init

initialize the interpolator with a set of sampling points

# $56 \quad numerical-methods/interpolation/@RegularizedInterpolator$

## 56.1 RegularizedInterpolator2

class for regularized interpolation on an unstructures mesh (
 interpolation)

#### 56.2 init

initialize the interpolator with a set of point samples

# 57 numerical-methods/interpolation/@RegularizedInterpolator

## 57.1 RegularizedInterpolator3

class for regularized interpolation (Tikhonov) on a triangulation (unstructured mesh)

## 57.2 init

initialize the interpolator with a set of sampling points

# 58 numerical-methods/interpolation

#### 58.1 IDW

spatial averaging by inverse distance weighting

### **58.2** IPoly

polynomial interpolation class

### 58.3 IRBM

# 58.4 ISparse

sparse interpolation class

### 58.5 Inn

nearest neighbour interpolation

## 58.6 Interpolator

 ${\tt interpolator \ super-class}$ 

fprintf(1,'Progress: %f%% %fs\n',100\*
 idx/size(Xt,1),t);

## 58.7 fixnan

fill nan-values in vector with gaps

#### 58.8 idw1

spatial average ny inverse distance weighting

### 58.9 idw2

spatial average by inverse distance weighting

#### 58.10 inner2outer

linear interpolation of segment mit point to grid points at segment ends assumes equal grid spacing

### 58.11 inner2outer2

interpolate from element (segment) centres to edge points

# 58.12 interp1\_limited

interpolate values, but not beyond a certain distance
this function is idempotent, i.e. it will not extrapolate over into
 gaps
exceedint the limit and thus not spuriously extend the series when
 called a second time on the same data

# 58.13 interp1\_man

interpolate

### 58.14 interp1\_save

make interpolation save to round off errors
the matlab internal interpolation suffers from rounding errors,
 which
are unacceptable when values of X and Y are large (for example UTm
 coordinates)
this normalization prevents this

## 58.15 interp1\_slope

quadratic interpolation returning value and derivative(s)

## 58.16 interp1\_smooth

## 58.17 interp1\_unique

matlab fails to interpolate, when x values are not unique this function makes the values unique before use

## 58.18 interp2\_man

nearest neighbour interpolation in two dimensions

## 58.19 interp\_angle

interpolate an angle

## 58.20 interp\_fourier

interpolation by the fourier method

# 58.21 interp\_fourier\_batch

batch interpolation by the fourier interpolation

### 58.22 interp\_sn

```
interpolate along streamwise coordinates
This gives similar result to setting aspect ratio for sN to
   infinity,
but not quite,as the input point set is not dense (scale for sN to
   infinity does not work)
        sdx = sdx(sdx_);
```

## 58.23 interp\_sn2

 ${\tt interpolation} \ {\tt in} \ {\tt streamwise} \ {\tt coordinates}$ 

# 58.24 interp\_sn3

# 58.25 interp\_sn\_

# 58.26 limit\_by\_distance\_1d

```
smooth subsequent values along a curve such that v(x0+dx) < v(x0) + (ratio-1)*dx if v is the edge length in a resampled polygon, then v_i/v_i+1) < ratio ratio^1 = exp(a*1)
```

# 58.27 resample1

interpolation along a parametric curve with variable step width

# 58.28 resample\_d\_min

resample a function

## 58.29 resample\_vector

resample a track so that velocity vectors do not run into each other  $% \left( 1\right) =\left( 1\right) \left( 1\right)$ 

# 58.30 test\_interp1\_limited

### 59 numerical-methods

### 59.1 inverse\_complex

# 60 numerical-methods/ode

## 60.1 bvp2\_check\_arguments

# 60.2 bvp2c

```
solve system of non-linear second order odes (in more than one
   variable)
as boundary value problems

odefun provides ode coefficients c:
c(x,1) y''(x) + c(x,2) y'(x) + c(x,3) y = c(x,4)
   c_1 y" + c_2 y' + c_3 y + c_4 = c_4

subject to the boundary conditions
bcfun provides v and p and optionally q, so that:

b_1 y + b_2 y' = f
   q(x,1)*( p(x,1) y_1(x) + p(x,2) y_1'(x)
   + q(x,2)*( p(x,1) y_r(x) + p(x,2) y_r'(x) = v(x)

where q weighs the waves travelling from left to right and right to
   left (default [1 1])
```

### 60.3 bvp2c2

```
solve second order boundary value problem via roots of the
   characteristic
polynomial
```

input:

```
x : [nx1] discretized domain
    n : number of vertices
    nxc = n-1 : number of segments
```

```
bc : struct : boundary condition
    bc.p(1)*y(0) + bc.pd(2)*y'(0) = bc.val(1)
    bc.p(2)*y(L) + bc.pd(2)*y'(L) = bc.val(2)

output:
A : [2*nxc x 2*ns] disrcretisation matrix
rhs : [2*nxc x 1] right hand size

y = A^-1 rhs
```

### 60.4 bvp2fdm

```
solve system of non-linear second order odes (in more than one
   variable)
as boundary value problems by the finite difference method

odefun provides ode coefficients c:
c(x,1) y''(x) + c(x,2) y'(x) + c(x,3) y = c(x,4)
c_1 y" + c_2 y' + c_3 y + c_4 = 0

subject to the boundary conditions
bcfun provides v and p and optionally q, so that:

b_1 y + b_2 y' = f
   q(x,1)*( p(x,1) y_1(x) + p(x,2) y_1'(x)
   + q(x,2)*( p(x,1) y_r(x) + p(x,2) y_r'(x) = v(x)

where q weighs the waves travelling from left to right and right to
   left (default [1 1])
```

### 60.5 bvp2wavetrain

solve second order boundary value problem by repeated integration

#### 60.6 bvp2wavetwopass

two pass solution for the linearised wave equation solve first for the wave number k, and then for y

## 60.7 ivp\_euler\_forward

solve intial value problem by the euler forward method

## 60.8 ivprk2

solve initial value problem by the two step runge kutta method

#### 60.9 ode2\_matrix

transformation matrix of second order ode to left and right going wave

```
c = odefun(x)
c1 y'' + c2' y + c3 y == 0
y = y_p + y_m, left and right going wave
d/dx [y_p, y_m] = A*[y_m, y_p]
```

### 60.10 ode2characteristic

second order odes transmittded and reflected wave

# 60.11 step\_trapezoidal

single trapezoidal step

## 60.12 $test_bvp2$

# 61 numerical-methods/optimisation

# 61.1 armijo\_stopping\_criterion

 ${\tt armijo} \ {\tt stopping} \ {\tt criterion} \ {\tt for} \ {\tt optimizations}$ 

### 61.2 astar

astar path finding alforithm

### 61.3 binsearch

binary search on a line

#### 61.4 bisection

bisection

### 61.5 box1

test objective function for optimisation routines

## 61.6 box2

## 61.7 cauchy

# 61.8 cauchy2

solve non-linear system by cuachy's method slower than quadratic optimisation, but does not require a hessian fun : objective function, returns

f : scalar, objective function value

g : nx1, gradient
x : nx1, initial position

opt : options

### 61.9 directional\_derivative

directional (projected) derivative
d : derivative, highest first
p : series expansion around x0

### 61.10 dud

optimization by the dud algorithm

### 61.11 extreme3

```
extract maxima by quadratic approximation from sampled function val
    (t)
intended to be called after [mval, mid] = max(val) for refinement
    of
locatian and maximum

input
t    : sampling time (uniformly spaced)
v    : values at sampling times
ouput:
tdx    : index where extremum should be computed
t0     : location of the extremum
val0    : value of extremum
v'(dt0) = 0 and v''(dt0) determines type of extremum
```

# 61.12 extreme\_quadratic

### 61.13 ftest

## 61.14 fzero\_bisect

# 61.15 fzero\_newton

### 61.16 grad

numerical gradient

### 61.17 hessian

numerical hessian

# 61.18 hessian\_from\_gradient

numerical hessian from gradient

# 61.19 hessian\_projected

numerical hessian projected to one dimenstion

### 61.20 line\_search

bisection routine

# 61.21 line\_search2

bisection method

fun : objective funct
x0 : start value

 ${\tt f0}$  : objective function value at  ${\tt x0}$ 

g : gradient at x0

 $\ensuremath{\mathtt{p}}$  : search direction from x0 (p = g for steepest descend)

h : initial step length (default 1)

 $\begin{array}{lll} \mbox{1b} & : \mbox{lower bound for } x \\ \mbox{up} & : \mbox{upper bound for } x \end{array}$ 

## 61.22 line\_search\_polynomial

polynomial line search
fun : objective funct
x0 : start value
f0 : objective function value at x0
g : gradient at x0
dir : search direction from x0 (p = g for steepest descend)
h : initial step length (default 1)
lb : lower bound for x
up : upper bound for x

# 61.23 line\_search\_polynomial2

cubic line search
fun : objective funct
x0 : start value
f0 : objective function value at x0
g : gradient at x0
dir : search direction from x0 (p = g for steepest descend)
h : initial step length (default 1)
lb : lower bound for x
up : upper bound for x

### 61.24 line\_search\_quadratic

quadratic line search
fun : objective funct
x0 : start value
f0 : objective function value at x0
g : gradient at x0
dir : search direction from x0 (p = g for steepest descend)
h : initial step length (default 1)
lb : lower bound for x
up : upper bound for x

### 61.25 line\_search\_quadratic2

quadratic line search

### 61.26 line\_search\_wolfe

line search by wolfe method
c.f.: OPTIMIZATION THEORY AND METHODS - Nonlinear Programming, Sun,
 Yuan

# 61.27 ls\_bgfs

least squares by the bgfs method

# 61.28 ls\_broyden

# 61.29 ls\_generalized\_secant

least squares by the secant method Barnes, 1965 Wolfe, 1959 Fletcher 1980, 6.3 seber 2003 gerber

### 61.30 nlcg

non-linear conjugate gradient
input:
x : nx1 start vectort

 ${\tt opt}$  :  ${\tt struct}$  options

 ${\tt fdx} \,:\, {\tt gradient} \,\, {\tt constraint}$ 

### 61.31 nlls

non-linear least squares

# 61.32 picard

picard iteration

# 61.33 poly\_extrema

extrema of a polynomial

# 61.34 quadratic\_function

evaluate quadratic function in higher dimensions

# 61.35 quadratic\_programming

optimize by quadratic programming  $% \left( 1\right) =\left( 1\right) \left( 1\right$ 

# 61.36 quadratic\_step

single step of the quadratic programming

### 61.37 rosenbrock

rosenbrock test function

# $61.38 \quad sqrt\_heron$

Heron's method for the square root

- 61.39 test\_directional\_derivative
- 61.40 test\_dud
- 61.41 test\_fzero\_newton
- $61.42 \quad test\_line\_search\_quadratic2$
- 61.43 test\_ls\_generalized\_secant
- 61.44 test\_nlcg\_6\_order
- 61.45 test\_nlls

$$f = w'*(p*abs(x-1).^4) + w'*(1-p)*abs(x-1).^2;$$

- 62 numerical-methods/pde
- 62.1 laplacian 2d\_fundamental\_solution

# 63 numerical-methods/piecewise-polynomials

### 63.1 Hermite1

hermite polynomial interpolation in 1d

## $63.2 \text{ hp2\_fit}$

fit a hermite polynomial
coefficients are derivative free
x0 : left point of first segment
x1 : right point of last segment
n : number of segments
x : sample x-value
val : sample y-value

c : coefficients (values at points, no derivatives)

# 63.3 hp2\_predict

prediction with pw hermite polynomial
c are values at support points

# 63.4 hp\_predict

predict with piecewise hermite polynomial

### 63.5 hp\_regress

fit piecewise hermite polynomial coefficients are values and derivatives

# 63.6 lp\_count

lagrangian basis for interpolation count number of valid samples

# $63.7 \quad lp\_predict$

lagrangian basis piecwie interpolation, predicor

- 63.8 lp\_regress
- 63.9 lp\_regress\_
- 64 regression/@PolyOLS
- 64.1 PolyOLS

class for polynomial least squares

64.2 coefftest

#### 64.3 detrend

detrending by polynomial regression

### 64.4 fit

fit a polynomial function like polyfit, but returns parameter error estimates TODO automatically activate scaleflag

64.5 fit\_

fit a polynomial function

# 64.6 predict

predict polynomial function values

64.7 predict\_

# 64.8 slope

slope by linear regression

# 65 regression/@PowerLS

# 65.1 PowerLS

class for power law regression

## 65.2 fit

fit a power law like polyfit, but returns parameter error estimates

# 65.3 predict

```
predict with power law
    S2 = diag((A*obj.C)*A');
    L = Y - S;
    U = Y + S;
```

# 65.4 predict\_

# 66 regression/@Theil

### 66.1 Theil

Kendal-Theil-Sen robust regression

#### 66.2 detrend

linear detrending of a set of samples by the Theil-Senn Slope

### 66.3 fit

fit slope and intercept to a set of sample with the Theil-Sen  $\tt method$ 

c : confidence interval c = 2\*ns\*normcdf(1) for ns-sigma
intervals

param : itercept and slope
P : confidence interval

# 66.4 predict

predict values and confidence intervals with the Theil-Sen method

# 66.5 slope

fit the slope with the Theil-Sen  $\ensuremath{\mathsf{method}}$ 

# 67 regression

linear and non-linear regression

### 67.1 Theil\_Multivariate

extension of the Theil-Senn regression to higher dimensions by means of the Gauss-Seidel iteration

# 67.2 areg

regression using the pth-fraction of samples with smallest residual

# 67.3 ginireg

gini regression

# 67.4 hessimplereg

```
hessian, gradient and objective function value of the simple regression  {\tt rhs} \, = \, {\tt p(1)} \, + \, {\tt p(2)} \, \, {\tt x} \, + \, {\tt eps}
```

#### 67.5 l1lin

solve ||Ax - b||\_L1 by means of linear programming

# 67.6 lsq\_sparam

parameter covariance of the least squares regression

```
fun : model function for predtiction
b : sample values
```

f(p) = b

p : parameter at point of evaluation (preferably optimum)

# 67.7 polyfitd

```
fit a polynomial of order n to a set of sampled values and sampled
   values
of the derivative

x0 must contain at least for conditioning as otherwise the
   intercept
cannot be determined
```

# 67.8 regression\_method\_of\_moments

fit linear function  $||a b x = y||_L2$  by the method of moments y+eps = alpha + beta\*x

# 67.9 robustling

fit a linear function by splitting the x-values at their median  $(med(y\_left) - med(y\_right))/(med(x\_left)-med(x\_right))$  this approach performs poorly compared to the theil-senn operator

#### 67.10 theil2

Theil senn-estimator for two dimensions (glm)

# 67.11 theil\_generalised

generalization of the Theil-Senn operator to higher dimensions,
for arbitrary functions such as polynomials and multivariate
 regression
either higher order polynomials or glm
c.f. "On theil's fitting method", Pegoraro, 1991

## 67.12 total\_least\_squares

total least squares

# 67.13 weighted\_median\_regression

weighted median regression c.f. Scholz, 1978

# 68 set-theory

### 68.1 issubset

test if set B is subset of A in O(n)-runtime

A : first set
B : second set

P : set of primes (auxiliary)

# 69 signal-processing

# 69.1 acf\_effective\_sample\_size

effective sample size from acf

# 69.2 acf\_genton

autocorrelation function

## 69.3 acfar1

Autocorrelation function of the finite AR1 process

```
a_k = 1/(n-k) sum x_ix_i+1 + (xi + xi+k)mu + mu^2
= r^k + 1/n sum_ij + 1/n
pause
```

### $69.4 \quad acfar1_2$

autocorrelation of the ar1 process

# 69.5 acfar2

impulse response of the ar2 process

### $69.6 \quad acfar2_{-2}$

autocorrelation of the ar2 process  $X_i + a1 X_{i-1} + a2 X_{i-2} = 0$ 

# 69.7 ar1\_cutoff\_frequency

# 69.8 ar1\_effective\_sample\_size

effective sample size correction for autocorrelated series

# $69.9 \quad ar1\_mse\_mu\_single\_sample$

standard error of a single sample of an ar1 correlated process

# $69.10 \quad ar1\_mse\_pop$

variance of the population mean of a single realisation around zero  ${\tt E[(mu_N-0)^2] = E[mu_N^n]}$ 

### 69.11 ar1\_mse\_range

 ${\tt mean}$  standard error of the  ${\tt mean}$  of a range of values taken from an ar1 process

### 69.12 ar1\_spectrum

spectrum of the ar1 process

## 69.13 ar1\_to\_tikhonov

convert ar1 correlation to tikhonovs lambda

#### $69.14 \quad ar1\_var\_factor$

```
variance correction factor for an autocorrelated finite process n : [1 .. inf] population size m : [1 .. n] samples size rho : [ -1 < \text{rho} < 1 (for convergence) ] correlation of samples
```

#### 69.15 ar1\_var\_factor\_

variance of an autocorrelated finite process

## $69.16 \quad ar1\_var\_range2$

```
variance of sub sample starting at the end of the series from the finite length first order autocorrelated process s2 = 1/m^2 \ sum\_i^m \ sum\_j^m \ rho^-|i-j|
```

### 69.17 ar1delay

# 69.18 ar1delay\_old

autocorrelation of the residual

#### 69.19 ar2conv

```
coefficients of the ar2 process determined from the two leading correlations of the acf [1,r1,r2,...]
```

### 69.20 ar2dof

effective samples size for the ar2 process

# 69.21 ar2param

ar2 parameter estimation from first two terms of acf
acf = [1 a1 a2 ...]

# 69.22 asymwin

creates asymmetrical filter windows filter will always have negative weights

#### 69.23 autocorr\_fft

autocorrelation function

# 69.24 bandpass

bandpass filter

# 69.25 bandpass 2

bandpass filter

#### 69.26 bartlett

```
Effective sample size factor for bartlett window c.f. thiebaux c.f spectral analysis-jenkins, eq. (6.3.27) c = acf note: results seams always to be 1 tac too low T : reduction factor for dof for ar1 with a = rho^k = \exp(-k/L), T = 2L
```

# 69.27 bartlett\_spectrogram

bartlet spectrogramm TODO sliding window

### 69.28 bin1d

bin values of  $\boldsymbol{v}$  sampled at  $\boldsymbol{x}$  into bins bounded by "edges" apply function  $\boldsymbol{v}$  to it

### 69.29 bin2d

```
bin values of V sampled at X and Y into the grid structured grid ex
    ,ey
apply function func to all walues in the bin
func = mean : default
func = sum : non-normalized frequency histogram in 2D
```

## 69.30 binormrnd

generate two correlated normally distributed vectors

# $69.31 \quad conv1_man$

convolutions with padding

### 69.32 conv2\_man

convolution in 2d

### 69.33 conv2z

### 69.34 conv30

convolve with rectangular window of length  $\boldsymbol{n}$  circular boundaries

69.35 conv\_

convolution of a with b

### 69.36 conv\_centered

convolve x with filter window f
when length of f is even, this guarantees a symmetric result (no
 off by on
displacement) by making the length of f odd at first

69.37 convz

# 69.38 cosexpdelay

## 69.39 csmooth

smooth recursively with [1,2,1]/4 kernel

# 69.40 daniell\_window

Daniell window for smoothing the power spectrum c.f. Daniell 1946
Bloomfield 2000
meko 2015

### 69.41 danielle\_window

danielle fourier window

# 69.42 db2neper

convert decibel to neper

# 69.43 db2power

power ratio from db

# 69.44 derive\_danielle\_weight

## 69.45 derive\_limit\_0\_acfar

# 69.46 detect\_peak

detect peaks in a vector requires function value to fall to p\*max before new value is allowed

# 69.47 digital\_low\_pass\_filter

design coefficients of a low pass filter with specified cut of
 frequency
and sampling period
alalogue low pass with pole at s=-omega\_c=1/tau=1/RC
Ha = tau/(tau + s) = 1/(1 + omega\_c\*s)

# 69.48 doublesum\_ij

double sum of r^i

# 69.49 effective\_sample\_size\_to\_ar1

convert effective sample size to ar1 correlation

# 69.50 filt\_hodges\_lehman

#### 69.51 filter1

filter along one dimension

#### 69.52 filter2

filter columns of x (matlab does only support vector input)

## 69.53 filter\_

invalidate values that exceed n-times the robust standard deviation

### 69.54 filteriir

filter adcp t-n data over time

v : nz,nt : values to be filtered
H : nt,1 : depth of ensemble

 ${\tt last} \ : \ {\tt nt,1} \ : \ {\tt last} \ {\tt bin} \ {\tt above} \ {\tt bottom} \ {\tt that} \ {\tt can} \ {\tt be} \ {\tt sampled} \ {\tt without}$ 

side lobe interference

nf : scalar : number of reweighted iterations

#### when samples

 distance to bed is reference (advantageous for near-bed suspended transport) TODO for wash load: distance to surface is more relevant interpolate depending on  $\boldsymbol{z}$ 

when depth changes, neighbouring indices do not correspond to same
 relative position in the water column
relative possition in the colum (s-coordinate) smoothes values
near the bed: absolute distance to bed is chosen
near surface: absolute distance to surface is chosen
-> cubic transformation of index

faster and avoid alising (smoothing along z)
 resample ensemble to same number of bins in S -> filter ->
 resample back
 use nonlinear transform z-s coordinates
-> resampling has to be local (Hi -> H-filtered)

filtered profile coordinates to sample coordinates

zf -> zi (special transform)

corresponding indices and fractions

filtration step (update of hf and vf)

sample coordinates to updated profile coordinates

(the inverse step is actually not necessary)

write filtered value

### 69.55 filterp

### 69.56 filterp1

fir filter with some fancy extras

#### 69.57 filterstd

## 69.58 firls\_man

design finite impulse response filter by the least squares method

# 69.59 flattopwin

the flat top window

# 69.60 frequency\_response\_boxcar

frquency response of a boxcar filter

# 69.61 freqz\_boxcar

frequncy response of a boxcar filter

# 69.62 gaussfilt1

filter data series with a gaussian window

# 69.63 hanchangewin

hanning window for change point detection

# 69.64 hanchangewin2

nanning window for chage point detection

# 69.65 hanwin

hanning filter window

# 69.66 hanwin\_

hanning filter window

# 69.67 highpass

high pass filter

# 69.68 kaiserwin

kaiser filter window

# 69.69 kalman

Kalman filter

# 69.70 lanczoswin

Lanczos window

# 69.71 last

lake tail, but for matrices

# 69.72 lowpass

low pass filter

# 69.73 lowpass 2

design low pass filter with cutoff-frequency f1

# 69.74 lowpass\_iir

iir-low pass

# 69.75 lowpass\_iir\_symmetric

two-sided iir low pass filter (for symmetry)

# 69.76 lowpassfilter 2

low-pass filter of data

### 69.77 maxfilt1

### 69.78 meanfilt1

moving average filter with special treatment of the boundaries

### 69.79 medfilt1\_man

moving median filter, supports columnwise operation

# 69.80 medfilt1\_man2

moving median filter with special treatment of boundaries

# $69.81 \quad medfilt 1\_padded$

median filter with padding

### 69.82 medfilt1\_reduced

median filter with padding

# $69.83 \quad mid\_term\_single\_sample$

variance of single sample, mid term

# 69.84 minfilt1

### 69.85 mu2ar1

error variance of the mean of the finite length ar1 process

(mu)^2 = (sum epsi)^2 = sum\_i sum\_j eps\_i eps\_j = sum\_ii(rho,n)/n^2 this has the limit s^2 for rho->1

# 69.86 mysmooth

### 69.87 nanautocorr

autocorrelation with nan-values

## 69.88 nanmedfilt1

medfilt1, skipping nans

# 69.89 neper2db

convert neper to db

# 69.90 peaks\_man

peaks of a periodogram

# 69.91 polyfilt1

```
polynomial filter,
can be achieved by iteratively processing the data with
a mean (zero-order) filter
```

# 69.92 qmedfilt1

medfilt1, after fitting a quadratic polynomial

## 69.93 randar1

```
generate random ar1 process
e1 = randar1(sigma,p,n,m)
```

### 69.94 randar1\_dual

draw random variables of two corrlated ar1 processes

### 69.95 randar2

generate ar2 process

# 69.96 randarp

randomly generate the instance of an ar-p process

# 69.97 range\_window

range of values within a certain range of indices (window)

# 69.98 rectwin

rectangular window

### 69.99 recursive\_sum

# 69.100 select\_range

# $69.101 \quad smooth 1 d\_parametric$

smooth position of p0=x0,y0 between p1=x1,y1 and p2=x2,y2, so that distance to p1 and p2 becomes equal and the chord length remains the same

### 69.102 smooth2

smooth vectos of X

# $69.103 \quad smooth\_man$

# 69.104 smooth\_parametric

smooth a parametric function given in x-y coordinates
 matvec2x2(R,[dxc;dyc])

# 69.105 smooth\_parametric2

parametrically smooth the curve

# $69.106 \quad smooth\_with\_splines$

### 69.107 smoothfft

filter with fast fourier transform

# 69.108 spectrogram

spectrogram

# $69.109 \quad std\_window$

moving block standard deviation

# $69.110 \quad sum\_i\_lag$

sum of ar1 matrix with lag
sum\_i=1^n rho^|i-k|

# 69.111 sum\_ii

sum of ar1 matrix
sum\_i=1^n sum\_j=1^n rho^|i-j|
this is for the variance, take square root for the standard
 deviation factor

# $69.112 \quad sum_ii_$

# 69.113 sum\_ij

# 69.114 sum\_ij\_

 $69.115 \quad sum\_ij\_partial\_$ 

69.116 sum\_multivar

sum of matrix entries of bivariate ar1 process

69.117 test\_acfar1

69.118 test\_acfar1\_2

69.119 test\_acfar1\_3

69.120 test\_acfar1\_4

 $69.121 \quad test\_acfar2$ 

69.122 test\_ar1\_var\_factor

69.123 test\_ar1\_var\_factor\_2

 $69.124 \quad test\_ar1\_var\_mu\_single\_sample$ 

- $69.125 \quad test\_ar1\_var\_pop$
- $69.126 \quad test\_ar1\_var\_pop\_1$
- 69.127 test\_ar1delay
- 69.128 test\_bivariate\_covariance\_term
- 69.129 test\_convexity
- 69.130 test\_lanczoswin
- 69.131 test\_madcorr
- 69.132 test\_randar1
- 69.133 test\_randar1\_multivariate
- 69.134 test\_randar2

69.135	test_sum_ij
69.136	$test\_sum\_multivar$
69.137	${ m test\_trifilt1}$
69.138	$test\_wautocorr$
69.139	$test\_wavelet\_transform$
69.140	${ m test\_wordfilt}$
69.141	$test\_xar1\_mid\_term$
69.142	$tikhonov\_to\_ar1$

69.143 trapwin

trapezoidal filter window

of the ar1 process

convert coefficient of the tikhonov regularization to correlatioon

### 69.144 trifilt1

filter with triangular window

### 69.145 triwin

triangular filter window

### 69.146 triwin2

triangular filter window

### 69.147 varar1

error variance of a single sample of a finite length ar1 process with respect to the mean, averaged over the population

# 69.148 welch\_spectrogram

welch spectrogram

## 69.149 wfilt

filter with window

# 69.150 winbandpass

filter with bandpass

# 69.151 window\_make\_odd

### 69.152 winfilt0

filter with window

# 69.153 winlength

window length for desired cutoff frequency
power at fc is halved
H(wf) = 1/sqrt(2) H(f)
if the filter window were used as a low pass filter
note: the user should prefer a windowed ideal low pass filter
TODO, relate this to DOF

### 69.154 wmeanfilt

mean filter with window

# 69.155 wmedfilt

median filter with window

### 69.156 wordfilt

weighted order filter

# 69.157 wordfilt\_edgeworth

weighed order filter

### 69.158 xar1

# $69.159 \quad xcorr_man$

cross correlation of two sampled ar1 processes

# 70 sorting

# 70.1 sort2

sort two numbers

# $70.2 \quad sort2d$

sort elements of matrix in  ${\tt X}$  returns row and column index of sorted values

# 71 special-functions

# 71.1 bessel\_sphere

spherical Bessel function of the first kind

# 71.2 digamma\_man

# 71.3 hankel\_sphere

spherical Hankel function for the far field (incident plane wave) first  ${\tt kind}$ 

### 71.4 hermite

probabilistic's hermite polynomial by recurrence relation

input :
n : order
x : value

output:
f : H\_n(x)

 $df : d/dx H_n(x)$ 

# 71.5 legendre\_man

legendre polynomials

# 71.6 neumann\_sphere

spherical Neumann function
Bessel function of the second kind

# 72 statistics

### $72.1 \quad atan\_s2$

stadard deviation of the arcus tangens by means of taylor expansion

# 72.2 beta\_mode\_to\_parameter

transform modes (mean and sd) to paramets of the beta function

# 72.3 coefficient\_of\_determination

# 72.4 conditional\_expectation\_normal

# 72.5 correlation\_confidence\_pearson

confience intervals of the correlation coefficient c.f. Fischer 1921

# 73 statistics/distributions

### 73.1 PDF

class for quasi-distributions from a set of sampling points

# $73.2 \quad binorm\_separation\_coefficient$

separation coefficient of a bimodal normal distribution

### 73.3 binormcdf

bio-modal gaussian distribution

### 73.4 binormfit

 $\hbox{fit sum of to normal distribution to a histogram}\\$ 

# 73.5 binormpdf

# 73.6 edgeworth\_cdf

edgeworth expansion of an unknown cumulative distribution with mean mu, standard deviation sigma, and third and fourth cumulants c.f. Rao 2010

## 73.7 edgeworth\_pdf

probability density of and unknown distribution
with mean mu, standard deviation sigma, and third and fourth
 cumulants
c.f. Rao 2010

## 73.8 logn\_mode2param

transform modes (mu,sd) to parameters of the log normal distribution  $% \left( 1\right) =\left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left($ 

## $73.9 logn_param2mode$

transform parameters to mode (mu, sd) for the  $\log$  normal distribution

# $73.10 \quad lognpdf_{-}$

log normal distribution called by modes rather than parameters

## 73.11 pdfsample

pdf from sample distribution
Note: better use kernal density estimates

#### 73.12 t2cdf

 $\hbox{\tt Hotelling's $T$-squared cumulative distribution}\\$ 

#### 73.13 t2inv

inverse of Hotelling's T-squared cumulative distribution

#### 74 statistics

# 74.1 example\_standard\_error\_of\_sample\_quantiles

#### 74.2 f\_var\_finite

reduction of variance when sampling from a finite population without replacement

# 74.3 gamma\_mode\_to\_parameter

transform modes (mu,sd) to parameters of the gamma distribution

## 74.4 gaussfit3

## 74.5 gaussfit\_quantile

## 74.6 hodges\_lehmann\_correlation

```
hodges_lehmann correlatoon coefficient
c.f. Shamos 1976
c.f. Bickel and Lehmann 1976
c.f. rousseeuw 1993
c.f. Shevlyakov 2011
```

## 74.7 hodges\_lehmann\_dispersion

```
dispersion determined by the hodges lehman method asymptotic efficiency of dispersion estimates: standard deviation: E(s - hat \ s)/s = 2/sqrt(2 \ n) ~ 0.707/sqrt(n) (100%) hodges lehmann dispersion E(s-hat \ s)/s = (pi/3)^2/(sqrt(2 \ n)) ~ 0.775/sqrt(n) (91%)
```

mad  $E(s-\hat s)/s \sim 1.17 \text{ s/sqrt(n)}$ (60%)

- c.f. Shamos 1976
- c.f. Bickel and Lehmann 1976
- c.f. rousseeuw 1993

nb: rousseeuw uses the 25th percentile, which is more efficient for small sample sizes

# 75 statistics/information-theory

#### 75.1 akaike\_information\_criterion

akaike information criterion

serr : rmse of model prediction

n : effective sample size
k : number of parameters

c.f. akaike (1974)

c.f. sugiura 1978

## 75.2 bayesian\_information\_criterion

bayesian information criterion

# 76 statistics

76.1 kurtncdf

## 76.2 kurtnpdf

## 76.3 kurtosis\_bias\_corrected

bias corrected kurtosis

## **76.4** limit

limit a by lower and upper bound

# 76.5 logfactorial

approximate log of the factorial

# 76.6 loglogpdf

76.7 lognfit\_quantile

# 76.8 logskewcdf

76.9 logskewpdf

# 77 statistics/logu

# 77.1 lambertw\_numeric

lambert-w function

# 77.2 logtrialtcdf

pdf of a logarithmic triangular distribution

#### 77.3 logtrialtiny

```
inverse of the logarithmic triangular distribution
= (d F log(a) log(b) + a log(b) - b log(a) - d F log(a) log(c) - a
    log(c) + d F log(b) log(c) + b log(c) - d F log^2(b))/((log(a)
    - log(b)) W((a^(-1/(log(a) - log(b))) (b^(-log(c)/log(a) - 1/
    log(a)) c)^(-log(a)/(log(a) - log(b))) (-d F log^2(b) + a log(b
    ) + d F log(a) log(b) + d F log(c) log(b) - b log(a) - a log(c)
    + b log(c) - d F log(a) log(c)))/(log(a) - log(b)))
x = (d F log(a) log(b) + a log(b) - b log(a) - d F log(a) log(c) - a
    log(c) + d F log(b) log(c) + b log(c) - d F log^2(b))/((log(a)
    - log(b)) W((a^(-1/(log(a) - log(b))) (b^(-log(c)/log(a) - 1/log
    (a)) c)^(-log(a)/(log(a) - log(b))) (-d F log^2(b) + a log(b) +
    d F log(a) log(b) + d F log(c) log(b) - b log(a) - a log(c) + b
    log(c) - d F log(a) log(c)))/(log(a) - log(b))))
```

#### 77.4 logtrialtmean

mean of the logarithmic triangular distribution

#### 77.5 logtrialtpdf

density of the logarithmic triangular distribution

## 77.6 logtrialtrnd

#### 77.7 logtricdf

 $\hbox{\it cumulative distribution of the logarithmic triangular distribution}\\$ 

## 77.8 logtriinv

invere of the logarithmic triangular distribution

# 77.9 logtrimean

mean of the logarithmic triangular distribution

# 77.10 logtripdf

probability density of the logarithmic triangular distribution

## 77.11 logtrirnd

## 77.12 logucdf

probability density of the logarithmic uniform distribution

# 77.13 logucm

central moments of the log-uniform distribution

# 77.14 loguinv

inverse of the log-uniform distribution

# 77.15 logumean

mean of the log-uniform distribution

# 77.16 logupdf

pdf of the log uniform distribution

# 77.17 logurnd

random numbers following a log-uniform distribution

# 77.18 loguvar

variance of the log-uniform distribution

#### 77.19 medlogu

median of the log-uniform distribution

# 77.20 test\_logurnd

#### 77.21 tricdf

cumulative distribution of the log-triangular distribution

## 77.22 triinv

inverse of the triangular distribution

# 77.23 trimedian

median of the triangular distribution

# 77.24 tripdf

probability density of the triangular distribution

#### **77.25** trirnd

random numbers of the triangular distribution

# 78 statistics

#### 78.1 maxnnormals

expected maximum of n normal variables c.f. Wolperts this is the median, not the mean of the maximum! see median of gumbel

## 78.2 midrange

mid range of columns of X

# 78.3 minavg

solution of the minimum variance problem minimise the variance of the weighted sum of n-independent random variables with equal mean and individual variance

#### $78.4 \quad mode\_man$

# 79 statistics/moment-statistics

## 79.1 autocorr\_man3

autoccorrelation of the columns of X

## 79.2 autocorr\_man4

autocorrelation for x if x is a vector, or indivvidually for the columns of x if x is a matrix

c.f. box jenkins 2008 eq. 2.1.12

Note that it is faster to compute the acf in frequency space as done in the matlab internal function

#### 79.3 autocorr\_man5

autocorrellation of the columns of X

#### 79.4 blockserr

estimate the standard error of potetially sequentilly correlated data  $% \left( 1\right) =\left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left( 1\right)$ 

by blocking

block length should be sufficiently larger than correlation length and sufficiently smaller than data length

this uses a sliding block approach, which reduces the variation of the error estimate

#### 79.5 comoment

non-central higher order moments of the multivariate normal distribution

 $\ensuremath{\mathsf{c.f.}}$  Moments and cumulants of the multivariate real and complex Gaussian distributions

note : there seem to be some typos in the original paper, for  $x^4 cii^2$ , the square seems to be missing

mu : nx1 mean vector

C : nxn covariance matrix

k : nx1 powers of variables in moments

## 79.6 corr\_man

correlation of two vectors

#### 79.7 cov\_man

covariance matrix of two vectors

#### 79.8 dof

mininum number of support points for a polynomial of degree order in dim dimensions

# 79.9 edgeworth\_quantile

inverse edgeworth expansion c.f. cornis fisher 1937 c.f. Rao 2010 c.f. 2.50 in hall CHERNOZHUKOV 3.3

# 79.10 effective\_sample\_size

effective sample size of the weighted mean of uncorrelated data  $\ensuremath{\text{c.f.}}$  Kish

#### 79.11 f\_correlation

correction factor for standard error of the mean of n ar1-correlated iid samples

#### 79.12 f\_finite

reduction factor of standard error for sampling from a finite
 distribution
without replacement

#### 79.13 lmean

mean of x.^l, not of abs

#### **79.14** lmoment

1-moment of vector x

# 79.15 maskmean

mean of the masked values of X

## 79.16 masknanmean

#### 79.17 mean1

mean of x

## $79.18 \quad mean\_man$

mean and standard error of X

# 79.19 mse

mean squared error of residual vector res this is de-facto the std for an unbiased residual

## 79.20 nanautocorr\_man1

autocorrelation of a vector with nan-values

### 79.21 nanautocorr\_man2

autocorrelation of a vector with nan-values

#### 79.22 nanautocorr\_man4

compute autocorrelation for x if x is a vector, or indivvidually for the columns of x if x is a matrix box jenkins 2008 eq. 2.1.12 TODO nan is problematic!

Note that it is faster to compute the acf in frequency space as done in the matlab internal function

#### 79.23 nancorr

(co)-correlation matrix when samples a NaN

# 79.24 nancumsum

cumulative sum, setting nan values to zero

#### 79.25 nanlmean

mean of the 1-th power of the absolute value of  $\boldsymbol{x}$ 

#### 79.26 nanr2

coefficient of determination when samples are invalid

#### **79.27** nanrms

root mean square value when sample contains nan-values

# 79.28 nanrmse

root mean square error from vector of residuals this is de-facto the std for an unbiased residual

#### 79.29 nanserr

standard error of  $\boldsymbol{x}$  with respect to mean when  $\boldsymbol{x}$  contains nan values

#### 79.30 nanwmean

```
weighted mean
min_x sum w (x-mu)^2 => mu = sum(wx)/sum(w)
varargin can be dim
function [mu serr] = nanwmean(w,x)
```

#### 79.31 nanwstd

weighed standard deviation

# 79.32 nanwvar

```
weighted variance of columns, corrected for degrees of freedom (
    bessel)

s^2 = sum(w*(x-sum(wx)/sum(w))^2)/sum(w)
```

### 79.33 nanxcorr

#### 79.34 pearson

pearson correlation coefficient

## 79.35 pearson\_to\_kendall

conversion of pearson to kendall correlation coefficient c.f. Kruskal 1958

# 79.36 pool\_samples

pooled mean and standard deviation of several groups of different size, mean and standard deviation

## 79.37 qmean

trimmed mean

# 79.38 range\_mean

#### $79.39 \quad rmse_{-}$

root mean square error computed from a residual vector this is de-facto the std for an unbiased residual

## 79.40 serr

standard error of the mean of a set of uncorrelated samples

# 79.41 serr1

# 79.42 test\_qskew

# 79.43 test\_qstd\_qskew\_optimal\_p

# 79.44 wautocorr

autocorrelation for x if x is a vector, or indivvidually for the columns of x if x is a matrix samples can be weighted

c.f. box jenkins 2008 eq. 2.1.12

c.f. autocorr\_man4

Note that it is faster to compute the acf in frequency space as done in the matlab internal function  $% \left( 1\right) =\left( 1\right) +\left( 1\right$ 

#### 79.45 wcorr

correlation of two vectors when samples are weighted

## 79.46 wcov

covariance of two vectors when samples are weighted

## 79.47 wdof

effective degrees of freedom for weighted samples

### 79.48 wkurt

kurtosis with weighted samples

#### 79.49 wmean

```
weighted mean
min_x sum w (x-mu)^2 => mu = sum(wx)/sum(w)
varargin can be dim
function [mu serr] = wmean(w,x)
```

#### 79.50 wrms

weighted root mean square error

#### 79.51 wserr

weighted root mean square error

#### 79.52 wskew

skewness of a weighted set of samples

#### 79.53 wstd

weighed standard deviation

### 79.54 wvar

```
weighted variance of columns, corrected for degrees of freedom (
    bessel)
variance of the weighted sample mean of samples with same mean (but
    not necessarily same variance)
s^2 = sum (w^2(x-sum(wx)^2))
s2_mu : error of mean, s2_mu : sd of prediction
```

# 80 statistics

#### 80.1 nangeomean

## 80.2 nangeostd

geometric standard deviation ignoring nan-values

# 81 statistics/nonparametric-statistics

#### 81.1 kernel1d

X : ouput x axis bins
xi : samples along x
m : number of bins in X
fun : kernel function

pdf : propability density of xi

#### 81.2 kernel2d

kernel density estimate in two dimensions

## 82 statistics

## 82.1 normmoment

expected norm of  $x.^n$ , when values x in x are iid normal with mu and sigma

#### 82.2 normpdf2

pdf of the bivariate normal distribution

# 83 statistics/order-statistics

## 83.1 hodges\_lehmann\_location

Asymptotic rms efficency of location estimte:
mean:
1 s/sqrt(n)

hodges lehman: sqrt(pi/3)\*s ~ 1.0233 s/sqrt(n) median: pi/2 s/sqrt(n) ~ 1.25 s / sqrt(n)

#### 83.2 kendall

kendall correlation coefficient

# 83.3 kendall\_to\_pearson

convert kendall rank correlation coefficient to the person product
 moment
correlation coefficient

c.f. Kruska, 1985

#### $83.4 \mod 2sd$

transform median absolute deviation to standard deviation for normal distributed values

#### 83.5 madcorr

proxy correlation by median absolute deviation

# 83.6 median2\_holder

#### 83.7 median\_ci

median and its confidence intervals under assumption of normality  $se_me = sqrt(1/2 pi) 1.25331 * sd/sqrt(n)$ 

## 83.8 median\_man

median and confidence intervals c is a P value for the confidence interval, default is 0.95 (2-sigma) median of the colums of X

#### 83.9 mediani

index of median, if median is not unique, any of the values is  ${\it chosen}$ 

#### 83.10 nanmadcorr

proxy correlation by median absolute deviation

#### 83.11 nanwmedian

weighted median, skips nan-values

## 83.12 nanwquantile

weighted quantile, skips nan values

# 83.13 oja\_median

two dimensional oja median
note: the multivariate median is not unique

oja 1983, for extension to multivariate function, see chaudhri

#### 83.14 qkurtosis

kurosis computed for quantiles

Note : this is a measurement of shape-tailedness and yields the same value for the  $\,$ 

normal distribution as "kurtosis"

However, this is a separate statistic and hence requires different  $% \left( 1\right) =\left( 1\right) +\left( 1\right)$ 

methods for calculating P-values and hypothesis testing

#### 83.15 qmoments

moments estimated from quantiles

## 83.16 qskew

skewness estimated from quantiles

Note: this is a measurement of shape-symmetry and yields the same value for the skew-normal distribution as "skewness"

However, this is an own statistic and hence requires different methods for calculating P-values and hypothesis testing

# 83.17 qskewq

skewness estimated by quantiles

## 83.18 qstdq

proxy standard deviation determined by quantiles

# 83.19 quantile1\_optimisation

# 83.20 quantile2\_breckling

qunatile regression

## 83.21 quantile2\_chaudhuri

quantile regression

# 83.22 quantile 2\_projected

quantile in two dimensions

# $83.23 \quad quantile 2\_projected 2$

spatial qunatile for chosen direction

# 83.24 quantile\_envelope

# 83.25 quantile\_regression\_simple

simple quantile regression

## 83.26 ranking

ranking for spearman statistics

# 83.27 spatial\_median

c.f. Oja 2008
is this the same as the oja simplex median (c.f. small 1990)?

# 83.28 spatial\_quantile

spatial quantile

# 83.29 spatial\_quantile2

spatial quantile

# 83.30 spatial\_quantile3

spatial quantile

# 83.31 spatial\_rank

unsigned rank

# 83.32 spatial\_sign

spatial sign

# 83.33 spatial\_signed\_rank

signed rank

Note: this is only a true rank if  ${\tt X}$  is normal with zero mean, abitrary variance

## 83.34 spearman

spearman's product moment coefficient

# 83.35 spearman\_rank

# 83.36 spearman\_to\_pearson

conversion of spearman rank to person product moment correlation coefficient  $% \left( 1\right) =\left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left( 1\right) +\left( 1\right) \left( 1\right) \left($ 

#### 83.37 wmedian

weighted median

# 83.38 wquantile

weighted quantile

# 84 statistics

84.1 qstd

# 84.2 quantile\_extrap

# 85 statistics/random-number-generation

# 85.1 laplacernd

random number of laplace distribution

#### 85.2 randc

correlate to correlated standard normally distributed vectors

## 85.3 skewness2param

# $85.4 \quad skewpdf\_central\_moments$

## 85.5 skewrnd

random numbers of the skew normal distribution

#### 85.6 skewrnd2

random numbers of the skew normal distribution

## 86 statistics

#### 86.1 range

mid range

# 86.2 resample\_with\_replacement

# 87 statistics/resampling-statistics/@Jackknife

#### 87.1 Jackknife

class for leave out 1 (delete 1) Jackknife estimates

- note 1 : the 1-delete jackknife does not yield consistend estimates for all functions,
  - in particular it will perform poorly on robust estimation functions
  - this is overcome by the d-delete jacknife, where d has to exceed the breakdown point
  - of the estimating function, for example  $\operatorname{sqrt}(n)$  for the median
  - as this leads to unreasonably large number of repetitions, bootstrap
  - is recommended for large sample cases (or blocking for sequential data)
- note 2 : as a linearisation, jackknife underestimates the error variance in case of

dependence in the data

note 3 : studentisation and the leave out 1 jackknife are related note 4 : the double 1 sample jacknife performs iferior to the d1 jacknife  $\frac{1}{2}$ 

#### 87.2 estimated\_STATIC

jacknife estimate of mean, bias and standard error
theta0 : estimate from all samples
thetad : set of estimates obtained by leaving out one data point
 each
 last dimension of theta is assumed to be the jackknife
 dimension

#### 87.3 matrix1\_STATIC

matrix of estimation for leaving out two samples at a time

#### 87.4 matrix2

matrix of estimations for jacknive with two samples left out

# 88 statistics/resampling-statistics

## 88.1 block\_jackknife

## 88.2 jackknife\_moments

moments determined by the jacknife

func : function of interest on the samples (e.g. mean)

A : parameter matrix columns : parameters

rows : samples of the parameter sets

d : number of samples left out

## 88.3 moving\_block\_jackknife

blocked Jacknfife for autocorrelated data
sliding block, statistically more efficient but computationally
 expensive
note, number of blocks must be sufficiently large h ~ sqrt(n)? << n</pre>

#### 88.4 randblockserr

standard error of sequentilly correlated data by blocking
block length should be sufficiently larger than correlation length
and sufficiently smaller than data length
this uses a sliding block approach, which reduces the variation of
the error estimate
TODO this does not work, randomly picking samples does not reveal
the correlation

### 88.5 resample

resample a vector and apply function to it TODO, should be with replacement

n : number of samples
m : number of subsamples

cx : maximum number of combinations

## 89 statistics

## 89.1 scale\_quantile\_sd

scale factor for the standard deviation of the asymtpotic distibution of sample quantiles (for normal distribution) see cadwell, 1952

#### 89.2 sd\_sample\_quantiles

# 89.3 skewpdf

skew-normal distribution c.f. Azzalini 1985

## $89.4 trimmed_mean$

trimmed mean

#### 89.5 $ttest2_man$

two-sample t-test here posix return value standard: h=0 accepted, h=1 failed note: the matlab logic is inverse : h=1 accepted, h=0 failed two sided univariate t-test

#### 89.6 ttest\_man

two-sample t-test
unequal sample size
equal variance

## 89.7 ttest\_paired

paired t-test unequal sample size equal variance more powerfull than unpaired test, as long as correlation between  $\rm x1$  and  $\rm x2\,>\,0$ 

## 89.8 wgeomean

weighted geometric mean
function mu = wgeomean(w,x)

# 89.9 wgeovar

variance of the weighted geometric mean

## 89.10 wharmean

weighted harmonic mean

## 89.11 wharstd

## 89.12 wharvar

# 90 mathematics

mathematical functions of various kind

## 90.1 ternary\_diagram

# 91 test/master

 $91.1 \quad dat\_test\_lanczos\_3d\_k\_20\_n\_40$ 

# $91.2 \quad poisson2d\_blk$

# 91.3 qr\_implicit\_givens\_2

91.4	$spectral\_derivative\_2d$
91.5	$test\_2d\_eigensolver\_hydrogen$
91.6	$test\_2d\_refine$
91.7	$test\_3d\_eigensolver\_hydrogen$
91.8	${ m test\_FEM}$
91.9	$test\_Mesh\_3d$
91.10	${ m test\_arnoldi}$
91.11	${ m test\_arpackc}$
91.12	$test\_assemble$

 $91.13 \quad test\_assembly\_performance$ 

- 91.14 test\_bc\_one\_sided
- 91.15 test\_compare\_solvers
- 91.16 test\_complete
- $91.17 \quad test\_convergence$
- 91.18 test\_convergence\_b
- $91.19 \quad test\_df\_2d$
- 91.20 test\_eig\_algs
- 91.21 test\_eig\_inverse
- $91.22 \quad test\_eigs\_lanczos$
- 91.23 test\_eigs\_lanczos\_1

- $91.24 \quad test\_eigs\_lanczos\_2$
- 91.25 test\_eigs\_lanczos\_performance
- 91.26 test\_fdm
- $91.27 \quad test\_fdm\_d\_vargrid$
- 91.28 test\_fdm\_spectral
- 91.29 test\_fem
- 91.30 test\_fem\_1d
- 91.31 test\_fem\_1d\_higher\_order
- 91.32 test\_fem\_2d\_adaptive
- 91.33 test\_fem\_2d\_higher\_order

- $91.34 \quad test\_fem\_3d\_higher\_order$
- 91.35 test\_fem\_3d\_refine
- 91.36 test\_fem\_b
- 91.37 test\_fem\_derivative
- 91.38 test\_fem\_quadrature
- 91.39 test\_final
- 91.40 test\_fix\_substitution
- 91.41 test\_forward
- $91.42 \quad test\_get\_sparse\_arrays$
- 91.43 test\_harmonic\_oscillator

91.44	test_high_order_fdm_periodic_bo
91.45	$test\_hydrogen\_wf$
91.46	test_ichol
91.47	$test\_interpolation$
91.48	$test\_inverse\_problem$
91.49	$test\_it\_vs\_exact$
91.50	test_jama
91.51	$\mathrm{test}_{ extsf{-}\mathbf{j}}\mathrm{d}$

91.52  $test\_jdqz$ 

91.53 test\_lanczos\_2

- $91.54 \quad test\_lanczos\_biorthogonal$
- 91.55 test\_laplacian
- 91.56 test\_laplacian\_non\_uniform
- 91.57 test\_laplacian\_simple
- 91.58 test\_mesh\_2d\_uniform
- 91.59 test\_mesh\_2d\_uniform\_2
- 91.60 test\_mesh\_circle
- 91.61 test\_mesh\_generation
- 91.62 test\_mesh\_interpolate
- 91.63 test\_mg

91.64	test_minres_recycle
91.65	${ m test\_multigrid}$
91.66	$\mathbf{test\_nc}$
91.67	$test\_nonuniform\_symmetric$
91.68	$\mathbf{test\_pde}$
91.69	$\mathbf{test\_permutation}$
91.70	${ m test\_poison\_fem}$
91.71	${ m test\_polar}$

91.72 test\_potential

91.73 test\_powers

- 91.74 test\_precondition
- 91.75 test\_project\_rectangle
- 91.76  $test\_qr$
- 91.77 test\_quantum\_well
- 91.78 test\_radial\_adaptive
- 91.79 test\_radial\_confinement
- 91.80 test\_radial\_fixes
- 91.81 test\_refine\_2d
- 91.82 test\_refine\_2d\_b
- 91.83 test\_refine\_3d

91.84	$test\_refine\_structural$
91.84	test_renne_structural

91.85	test_regul	larisation
01.00		

91.86 test\_round\_off

 $91.87 \quad test\_schrdinger\_potentials$ 

91.88 test\_uniform\_mesh

91.89 test\_vargrid

92 test

 $92.1 \quad test\_gaussfit3$ 

92.2 test\_mtimes3x3

# 93 wavelet

#### 93.1 continuous\_wavelet\_transform

```
continuous wavelet transform follows "The Illustrated Wavelet Transform Handbook: Introductory Theory and \dots"
```

#### 93.2 cwt\_man

continuous fourier transform as of time of implmentation, the matlab interal cwt is affected by serious round-off errors and has issues with the scaling, which is not the case here

## 93.3 example\_wavelets

# 93.4 phasewrap

wrap the phase to +/- pi

## 93.5 test\_cwt\_man

## 93.6 test\_phasewrap

#### 93.7 test\_wavelet

### 93.8 test\_wavelet2

## $93.9 test_wavelet_analysis$

#### 93.10 test\_wavelet\_reconstruct

## $93.11 ext{test_wtc}$

#### 93.12 wavelet

wavelet windows

## 93.13 wavelet\_reconstruct

iverses wavelet transform for single frequency
(reconstruction of time series)
n : window lengths in multiples of filter period 1/f0

#### 93.14 wavelet\_transform

wavelet transform for single frequency n: window lengths in multiples of filter period 1/f0

## 94 mathematics

mathematical functions of various kind

# 94.1 wrapphase