R documentation

of all in '.'

October 11, 2025

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*.cf

Divide two cf objects by each other measurement by measurement

Description

Note that no complex arithmetic is used, real and imaginary parts are treated as seperate and indepenent, such that the real part of one is the divided by the real part of the other and similarly for the imaginary parts.

Usage

```
## S3 method for class 'cf'
cf1 * cf2
## S3 method for class 'cf'
cf1 / cf2
```

Arguments

```
cf1, cf2 cf_orig objects.
```

Details

Note that this is generally only allowed on bootstrap samples and mean values, although it makes sense in some exeptional circumstances. Don't use this function unless you're certain that you should!

Value

The value is

cf1/cf2.

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*.raw_cf

multiply two raw_cf objects

Description

multiply two raw_cf objects

Usage

```
## S3 method for class 'raw_cf'
cf1 * cf2
```

Arguments

cf1 first 'raw_cf' container with data and meta-data to be multiplied cf2 second 'raw_cf' container with data and meta-data to be multiplied

Value

```
raw_cf object with cf$data == cf1$data * cf2$data
```

+.cf

Arithmetically add correlators

Description

Arithmetically add correlators

Usage

```
## S3 method for class 'cf'
cf1 + cf2
```

Arguments

cf1, cf2 cf_orig objects.

Value

The value is

$$cf1 + cf2$$
.

-.cf

+.raw_cf

add two raw_cf objects

Description

add two raw_cf objects

Usage

```
## S3 method for class 'raw_cf'
cf1 + cf2
```

Arguments

cf1 first 'raw_cf' container to be added cf2 second 'raw_cf' container to be added

Value

```
raw_cf object with cf$data == cf1$data + cf2$data
```

-.cf

Arithmetically subtract correlators

Description

Arithmetically subtract correlators

Usage

```
## S3 method for class 'cf'
cf1 - cf2
```

Arguments

cf1, cf2 cf_orig objects.

Value

The value is

$$cf1 - cf2$$
.

-.raw_cf

-.raw_cf

add two raw_cf objects

Description

```
add two raw_cf objects
```

Usage

```
## S3 method for class 'raw_cf'
cf1 - cf2
```

Arguments

cf1 first 'raw_cf' container to be subtracted
cf2 second 'raw_cf' container to be subtracted

Value

```
raw_cf object with cf$data == cf1$data - cf2$data
```

/.raw_cf

divide two raw_cf objects

Description

```
divide two raw_cf objects
```

Usage

```
## S3 method for class 'raw_cf'
cf1 / cf2
```

Arguments

cf1 'raw_cf' container with data and meta-data to be the dividend cf2 'raw_cf' container with data and meta-data to be the divisor

Value

```
raw_cf object with cf$data == cf1$data / cf2$data
```

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add.cf

Arithmetically adds two correlation functions

Description

Arithmetically adds two correlation functions

Usage

```
add.cf(cf1, cf2, a = 1, b = 1)
```

Arguments

cf1, cf2 cf_orig object.

a, b Numeric. Factors that multiply the correlation function before the addition.

Since addition is associative, this operates also on the bootstrap samples and

these are thus not invalidated in the process.

Value

The value is

$$aC_1 + bC_2$$
.

add.raw_cf

add two raw_cf objects

Description

add two raw_cf objects

Usage

add.raw_cf(cf1, cf2,
$$a = 1$$
, $b = 1$)

Arguments

| cf1 | first 'raw_cf' container with data and meta-data |
|-----|--|
| cf2 | second 'raw_cf' container with data and meta-data |
| а | Numeric or complex, scaling factor applied to cf1. |
| b | Numeric or complex, scaling factor applied to cf2. |

Value

```
a*cf1$data + b*cf2$data
```

addConfIndex2cf 11

addConfIndex2cf

add a configuration index to an cf object

Description

add a configuration number index to cf object.

Usage

```
addConfIndex2cf(cf, conf.index)
```

Arguments

cf and object of class cf

conf. index a configuration index of the same length as cf.

Value

Returns an object of class cf equal to the input but with element conf. index added

Author(s)

Carsten Urbach, <urbach@hiskp.uni-bonn.de>

See Also

cf

Examples

```
data(samplecf)
conf.index <- c(1:1018)
samplecf <- addConfIndex2cf(samplecf, conf.index=conf.index)</pre>
```

addStat.cf

Combine statistics of two cf objects

Description

addStat.cf takes the raw data of two cf objects and combines them into one

Usage

```
addStat.cf(cf1, cf2)
```

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Arguments

| cf1 | the first of the two cf objects to be combined |
|-----|---|
| cf2 | the second of the two cf objects to be combined |

Details

Note that the two cf objects to be combined need to be compatible. Otherwise, addStat.cf will abort with an error.

Value

an object of class cf with the statistics of the two input cf objects combined

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

cf

Examples

```
data(samplecf)
## the following is not useful, but
## explains the usage
cfnew <- addStat.cf(cf1=samplecf, cf2=samplecf)</pre>
```

addStat.raw_cf

Extend statistics of an existing raw_cf container

Description

Extend statistics of an existing raw_cf container

Usage

```
addStat.raw_cf(cf1, cf2)
```

Arguments

| cf1 | raw_cf container with or without 'data' and 'meta' mixin |
|-----|--|
| cf2 | raw_cf container with or without 'data' and 'meta' mixin |

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Details

When either of cf1 or cf2 does not contain any data, the other object is returned. (allows empty raw_cf to be extended). If the dimensions (except for the measurements) of the data fields of the two containers match, they are concatenated along the measurement dimension.

Value

An object of S3 class raw_cf identical to the input object but with extended statistics.

alphas

compute alpha strong at given scale

Description

compute alpha strong (α_s) at given scale μ up to N3LO in PT in the RI' renormalisation scheme.

Usage

```
alphas(mu, nl = 3, lam0 = 0.25, Nc = 3, Nf = 2, use.cimpl = TRUE)
```

Arguments

mu the renormalisation scale μ in GeV

nl order in PT, range 0 to 3

lam0 Λ_{QCD} in GeV

Nc number of colours N_c , defaults to 3 Nf number of flavours N_f , default is 2

use.cimpl Use the C implementation instead of the R implementation, which might im-

prove speed.

Value

returns the value of alpha strong α_s at scale μ

Author(s)

Carsten Urbach, <curbach@gmx.de>, Vittorio Lubicz (of the original Fortran code)

See Also

zetazp

Examples

```
alphas(mu=2.0, nl=3)
```

```
analysis_gradient_flow
                        analysis_gradient_flow
```

Description

function to analyse the gradient flow output files generated by the tmLQCD software, see references.

Usage

```
analysis_gradient_flow(path, outputbasename, basename = "gradflow",
 read.data = TRUE, pl = FALSE, plotsize = 4, skip = 0, start = 0,
  scale = 1, dbg = FALSE)
```

Arguments

| path | string. path to data files |
|------------------------|--|
| ${\tt outputbasename}$ | string. basename of output files |
| basename | string. basename of input files, for example "gradflow" |
| read.data | $boolean.\ Indicates\ whether\ to\ read\ data\ fresh\ from\ data\ files\ or\ to\ use\ basename\ . \\ raw.\ gradflow\ .\ Rdatainstead$ |
| pl | boolean. If set to TRUE plots will be generated |
| plotsize | numeric. Plot sidelength, this is passed to tikz.init. |
| skip | integer. number of measurements to skip |
| start | integer. start value for time |
| scale | numeric. scale factor for the MD time, should be set to the stridelength (in units of trajectories or configurations) which was used to produce the gradient flow files, such that the distance between measurements can be interpreted correctly and the reported autocorrelation times scaled appropriately. |
| dbg | boolean. If set to TRUE debugging output will be provided. |
| | |

Value

Nothing is returned.

References

K. Jansen and C. Urbach, Comput. Phys. Commun. 180 (2009) 2717-2738

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|--|

Description

analysis_online is a function to analyse the online measurements and output files of the tm-LQCD software, see references. The function operates on a subdirectory either passed via rundir or automatically constructed from the various function arguments. Depending on which parts of the analysis are requested, this subdirectory is expected to contain onlinemeas.%06d files with online correlator measurements, output.data containing the plaquette and energy violation, amongst others and monomial-%02d.data with measurements of the extremal eigenvalues of the

Usage

```
analysis_online(L, Time, t1, t2, beta, kappa, mul, cg_col, evals_id, rundir,
  cg.ylim, type = "", csw = 0, musigma = 0, mudelta = 0, muh = 0,
  addon = "", skip = 0, rectangle = TRUE, plaquette = TRUE,
  dH = TRUE, acc = TRUE, trajtime = TRUE, omeas = TRUE, plotsize = 5,
  debug = FALSE, trajlabel = FALSE, title = FALSE, pl = FALSE,
  method = "uwerr", fit.routine = "optim", oldnorm = FALSE, S = 1.5,
  stat_skip = 0, omeas.samples = 1, omeas.stride = 1, omeas.avg = 1,
  omeas.stepsize = 1, evals.stepsize = 1, boot.R = 1500, boot.l = 2,
  outname_suffix = "", verbose = FALSE)
```

Arguments

| L | integer. spatial lattice extent |
|----------|--|
| Time | integer. temporal lattice extent |
| t1 | integer. initial time of fit range |
| t2 | integer. end time of fit range |
| beta | numeric. inverse squared gauge coupling |
| kappa | numeric. hopping parameter |
| mul | numeric. light sea twisted quark mass |
| cg_col | integer. column of CG iteration counts from output.data to use |
| evals_id | Integer. Monomial ID of the monomial for which eigenvalues are measured. Function will attempt to open monomial-%02d.data. |
| rundir | string. run directory. If not specified, run directory will be constructed automatically. See construct_onlinemeas_rundir for details. |
| cg.ylim | numeric. y-limits for CG iteration counts |
| type | string. Type specifier for the gauge action, this might be 'iwa' for Iwasaki, for example. |
| CSW | numeric. clover coefficient |
| musigma | numeric. average 1+1 sea twisted quark mass |
| | |

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mudelta numeric. splitting 1+1 sea twisted quark mass

muh numeric. "heavy" twisted mass in the case of a n_f=2+2 run

addon string. addon to output filenames

skip integer. number of initial measurements to skip in analysis

rectangle boolean. If true, rectangle plaquettes are analysed boolean. If true, square plaquettes are analysed

dH boolean. If true, delta H is analysed

acc boolean. If true, the acceptance rate is analysed trajtime boolean. If true, the time per trajectory is analysed

omeas boolean. If true, online measurements are analysed (onlinemeas.%06d)

plotsize numeric. size of plots being generated debug boolean. provide debug information

trajlabel boolean or string. If not FALSE, use as trajectory labels title bolean or string. If not FALSE, use as main title of plots

pl boolean. If set to TRUE plots will be generated

method string. method to compute errors, can be "uwerr", "boot" or "all"

fit.routine string. minimisation routine for chisq, can be "optim"

oldnorm boolean. If TRUE, the function assumes that the onlinemeas. %06d are in old

tmLQCD normalisation.

S numeric. S parameter of uwerr

stat_skip integer. By passing this parameter, the various timeseries plots will include

stat_skip measurements, but these will be skipped in the corresponding statistical analysis. This maybe useful, for example, to visualise thermalisation.

omeas.samples integer. number of stochastic samples per online measurement omeas.stride integer. stride length in the reading of online measurements omeas.avg integer. Block average over this many subsequent measurements.

omeas.stepsize integer. Number of trajectories between online measurements. Autocorrelation

times of online measurement data will be scaled by this factor.

evals.stepsize integer. Numer of trajectories between (strange-charm Dirac opertoar) eigen-

value measurements. Autocorrelation times of eigenvalues will be scaled by

this factor.

boot.R integer. number of bootstrap samples to use in bootstrap-based parts of analysis.

boot.1 integer. bootstrap block size outname_suffix string. suffix for output files

verbose boolean. If TRUE, function produces verbose output. #'

Value

a list is returned with all the accumulated results. Moreover, a PDF file with statistics and analytics is created and the results are written into .Rdata files. On the one hand, the result of the call to the onlinemeas function is written to onlineout.%s.Rdata, where %s is replaced with a label built from meta information based on the arguments above. On the other hand, summary data across many calls of this function is silently accumulated in the file omeas.summary.Rdata which contains the named list 'resultsum' with element names based on rundir.

avg.cbt.cf

References

K. Jansen and C. Urbach, Comput. Phys. Commun. 180 (2009) 2717-2738

avg.cbt.cf

average close-by-times in a correlation function

Description

"close-by-times" averaging replaces the value of the correlation function at t with the "hypercubic" average with the values at the neighbouring time-slices with weights 0.25, 0.5 and 0.25 $C(t^2) = 0.25$ C(t-1) + 0.5 C(t) + 0.25 C(t+1) where periodic boundary conditions are assumed in shift.cf

Usage

```
avg.cbt.cf(cf)
```

Arguments

cf

object of type cf

Value

Returns an object of class cf.

block.raw_cf

Block average correlation function data

Description

Block block_length sequential measurements of the correlation function together. This occurs, for example, when multiple stochastic noise vectors are used per measurement or multiple source locations. Alternatively, it can also be used to account for auto-correlations in the data. If the total number of measurements is not divisible by block_length, the last measurements are discarded.

Usage

```
block.raw_cf(cf, block_length)
```

Arguments

cf raw_cf object

block_length Integer, number of successive measurements to average over.

Value

cf raw_cf object with the data member reduced in its first dimension by a factor of block_length and restricted (at the end) to the number of measurements divisible by block_length.

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bootstrap.analysis

Performs a Bootstrap with Blocking Analysis of a Timeseries

Description

Performs a Bootstrap with Blocking Analysis of a Timeseries

Usage

```
bootstrap.analysis(data, skip = 0, boot.R = 100, tsboot.sim = "geom",
 pl = FALSE, boot.1 = 2)
```

Arguments

data a numerical vector containing the time series skip integer value providing the warm up phase length. boot.R number of bootstrap samples. See also boot, and tsboot. tsboot.sim the sim parameter of tsboot.

logical, indicating whether or not to plot the result. pl

boot.1 block length for blocked bootstrap.

Details

the routine will compute the error, the error of the error and the integrated autocorrelation time for different block size using a bootstrap analysis. The blocksize is systematically increased starting from 1 until (length(data)-skip)/blocksize < 20. Note that only data is kept in exact multiples of the block length.

Value

returns a data frame containing the mean value, the error approximation, the estimate of the error of the error, the value of tau int and the bias for all block sizes.

Author(s)

```
Carsten Urbach, <carsten.urbach@liverpool.ac.uk>
```

See Also

for an alternative way to analyse such time series see uwerr and computeacf

Examples

```
data(plaq.sample)
plaq.boot <- bootstrap.analysis(plaq.sample, pl=TRUE)</pre>
```

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| | | | | _ |
|----|-----|----|-----|------|
| bo | nt. | st | ran | . ct |

bootstrap a set of correlation functions

Description

bootstrap a set of correlation functions

Usage

```
bootstrap.cf(cf, boot.R = 400, boot.l = 2, seed = 1234, sim = "geom",
endcorr = TRUE)
```

Arguments

| cf | correlation matrix of class cf e.g. obtained with a call to extrac.obs. |
|---------|--|
| boot.R | number of bootstrap samples. |
| boot.1 | block size for autocorrelation analysis |
| seed | seed for the random number generation used for boostrapping. |
| sim | The type of simulation required to generate the replicate time series. The possible input values are '"fixed"' (block resampling with fixed block lengths of 'boot.l') and '"geom"' (block resampling with block lengths having a geometric distribution with mean 'boot.l'). Default is '"geom"'. See tsboot for details. |
| endcorr | A logical variable indicating whether end corrections are to be applied when |

'sim' is '"fixed"'. When 'sim' is '"geom"', 'endcorr' is automatically set to 'TRUE'; 'endcorr' is not used when 'sim' is '"model"' or '"scramble"'. See

tsboot for details.

Value

returns an object of class cf with bootstrap samples added for th correlation function called cf.tsboot. Moreover, the original average of cf is returned as cf0 and the bootstrap errors as tsboot.se. We also copy the input parameters over and set bootstrap.samples to TRUE.

Author(s)

```
Carsten Urbach, <curbach@gmx.de>
```

See Also

```
tsboot, jackknife.cf
```

Examples

```
data(samplecf)
samplecf <- bootstrap.cf(cf=samplecf, boot.R=99, boot.l=2, seed=1442556)
plot(samplecf, log=c("y"))</pre>
```

bootstrap.effectivemass

Computes effective masses with bootstrapping errors

Description

Generates bootstrap samples for effective mass values computed from an object of class cf (a correlation function)

Usage

```
bootstrap.effectivemass(cf, type = "solve")
```

Arguments

cf

a correlation function as an object of type cf, preferably after a call to bootstrap.cf. If the latter has not been called yet, it will be called in this function.

type

The function to be used to compute the effective mass values. Possibilities are "acosh", "solve", "log", "temporal", "shifted" and "weighted". While the first three assume normal cosh behaviour of the correlation function, "temporal" is desigend to remove an additional constant stemming from temporal states in two particle correlation functions. The same for "shifted" and "weighted", the latter for the case of two particle energies with the two particle having different energies. In the latter case only the leading polution is removed by removeTemporal.cf and taken into account here.

Details

A number of types is implemented to compute effective mass values from the correlation function:

```
"solve": the ratio C(t+1)/C(t) = \cosh(-m*(t+1))/\cosh(-m*t) is numerically solved for m. 
"acosh": the effective mass is computed from m = a\cosh((C(t-1)+C(t+1))/(2C(t))) Note that this definition is less tolerant against noise. 
"log": the effective mass is defined via m = \log(C(t)/C(t+1)) which has artifacts of the periodicity at large t-values. 
"temporal": the ratio [C(t)-C(t+1)]/[C(t-1)-C(t)] = [\cosh(-m*(t))-\cosh(-m*(t+1))]/[\cosh(-m*(t-1))-\cosh(-m(t))] is numerically solved for m(t).
```

"shifted": like "temporal", but the differences C(t)-C(t+1) are assumed to be taken already at the correlator matrix level using removeTemporal.cf and hence the ratio

```
[C(t+1)]/[C(t)] = [\cosh(-m*(t)) - \cosh(-m*(t+1))]/[\cosh(-m*(t-1)) - \cosh(-m(t))] is numerically solved for m(t).
```

"weighted": like "shifted", but now there is an additional weight factor w from removeTemporal.cf to be taken into account, such that the ratio

```
[C(t+1)]/[C(t)] = [\cosh(-m*(t)) - w*\cosh(-m*(t+1))]/[\cosh(-m*(t-1)) - w*\cosh(-m(t))]
```

is numerically solved for m(t) with w as input.

Value

An object of class effectivemass is invisibly returned. It has objects: effMass:

The computed effective mass values as a vector of length Time/2. For type="acosh" also the first value is NA, because this definition requires three time slices.

deffMass:

The computed bootstrap errors for the effective masses of the same length as effMass.

```
effMass.tsboot:
```

The boostrap samples of the effective masses as an array of dimension RxN, where R=boot.R is the number of bootstrap samples and N=(Time/2+1).

```
and boot.R, boot.1, Time
```

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

arXiv:1203.6041

See Also

```
fit.effectivemass, bootstrap.cf, removeTemporal.cf
```

Examples

```
data(samplecf)
samplecf <- bootstrap.cf(cf=samplecf, boot.R=99, boot.l=2, seed=1442556)
effmass <- bootstrap.effectivemass(cf=samplecf)
summary(effmass)
plot(effmass, ylim=c(0.14,0.15))</pre>
```

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| h + - + | . ~ |
|----------|--------|
| bootstra | p.gevp |

perform a bootstrap analysis of a GEVP

Description

perform a bootstrap analysis of a GEVP for a real, symmetric correlator matrix

Usage

```
bootstrap.gevp(cf, t0 = 1, element.order = 1:cf$nrObs,
   sort.type = "vectors", sort.t0 = TRUE)
```

Arguments

| cf | correlation matrix obtained with a call to extrac.obs. |
|---------------|--|
| t0 | initial time value of the GEVP, must be in between 0 and Time/2-2. Default is 1. |
| element.order | specifies how to fit the n linearly ordered single correlators into the correlator matrix. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Double indexing is allowed. |
| sort.type | Sort the eigenvalues either in descending order, or by using the scalar product of the eigenvectors with the eigenvectors at $t=t_0+1$. Possible values are "values", "vectors" and "det". The last one represents a time consuming, but in principle better version of sorting by vectors. |
| sort.t0 | for sort.type "vectors" use t_0 as reference or $t-1$. |

Details

Say something on "det" sorting method.

Value

```
Returns an object of class gevp with member objects:
```

cf.

The input data, if needed bootstrapped with bootstrap.cf.

res.gevp

The object returned from the call to gevp. For the format see gevp.

gevp.tsboot:

The bootstrap samples of the GEVP. For the format see gevp.

Author(s)

Carsten Urbach, <curbach@gmx.de>

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References

```
Michael, Christopher and Teasdale, I., Nucl.Phys.B215 (1983) 433, DOI: 10.1016/0550-3213(83)90674-0
Blossier, B. et al., JHEP 0904 (2009) 094, DOI: 10.1088/1126-6708/2009/04/094, arXiv:0902.1265
```

See Also

```
gevp, extract.obs, bootstrap.cf
```

Examples

```
data(correlatormatrix)
## bootstrap the correlator matrix
correlatormatrix <- bootstrap.cf(correlatormatrix, boot.R=99, boot.l=1, seed=132435)</pre>
## solve the GEVP
t0 <- 4
correlatormatrix.gevp <- bootstrap.gevp(cf=correlatormatrix, t0=t0, element.order=c(1,2,3,4))</pre>
## extract the ground state and plot
pc1 <- gevp2cf(gevp=correlatormatrix.gevp, id=1)</pre>
plot(pc1, log="y")
## determine the corresponding effective masses
pc1.effectivemass <- bootstrap.effectivemass(cf=pc1)</pre>
pc1.effectivemass <- fit.effectivemass(cf=pc1.effectivemass, t1=5, t2=20)</pre>
## summary and plot
summary(pc1.effectivemass)
plot(pc1.effectivemass)
## we can also use matrixfit with a special model for a principal
## correlators
pc1.matrixfit <- matrixfit(pc1, t1=2, t2=24, fit.method="lm", model="pc", useCov=FALSE,</pre>
                      parlist=array(c(1,1), dim=c(2,1)), sym.vec=c("cosh"), neg.vec=c(1))
summary(pc1.matrixfit)
plot(pc1.matrixfit)
## the same can be achieved using bootstrap.nlsfit
model <- function(par, x, t0, ...) {</pre>
 return(exp(-par[1]*(x-t0))*(par[3]+(1-par[3])*exp(-par[2]*(x-t0))))
ii < -c(2:4, 6:25)
fitres <- parametric.nlsfit(fn=model, par.guess=c(0.5, 1, .9),</pre>
                             y=pc1$cf0[ii], dy=pc1$tsboot.se[ii],
                             x=ii-1, boot.R=pc1$boot.R, t0=t0)
summary(fitres)
plot(fitres, log="y")
```

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Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input cf object and a generalised eigenvalue problem is solved then. This is the function to call. It will perform a bootstrap analysis.

Usage

```
bootstrap.hankel(cf, t0 = 1, n = 2, N = (cf$Time/2 + 1),
  t0fixed = TRUE, deltat = 1, Delta = 1, custom.indices = NA,
  submatrix.size = 1, element.order = 1)
```

Arguments

| cf | object of type cf |
|----------------|---|
| t0 | Integer. Initial time value of the GEVP, must be in between 0 and Time/2-n. Default is 1. Used when t0fixed=TRUE. |
| n | Integer. Size of the Hankel matrices to generate |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix |
| t0fixed | Integer. If set to TRUE, keep t0 fixed and vary deltat, otherwise keep deltat fixed and vary t0. |
| deltat | Integer. value of deltat used in the hankel GEVP. Default is 1. Used t0fixed=FALSE |
| Delta | integer. Delta is the time shift used in the Hankel matrix. |
| custom.indices | integer. Vector of indices to be using in cf instead of computing them from 'Delta' and 't0' |
| submatrix.size | Integer. Submatrix size to be used in build of Hankel matrices. Submatrix.size > 1 is experimental. |
| element.order | Integer vector. specifies how to fit the n linearly ordered single correlators into the correlator matrix for submatrix.size > 1. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Matrix elements can occur multiple times, such as c(1,2,2,3) for the symmetric case, for example. |

Details

```
See vignette(name="hankel", package="hadron")
```

Value

List object of class "hankel". The eigenvalues are stored in a numeric vector t0, the corresonding samples in t. The reference input time t0 is stored as reference_time in the returned list.

See Also

```
Other hankel: bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm(), gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()
```

Examples

```
data(correlatormatrix)
correlatormatrix <- bootstrap.cf(correlatormatrix, boot.R=99, boot.l=1, seed=132435)
t0 <- 4
correlatormatrix.gevp <- bootstrap.gevp(cf=correlatormatrix, t0=t0, element.order=c(1,2,3,4))
pc1 <- gevp2cf(gevp=correlatormatrix.gevp, id=1)
pc1.hankel <- bootstrap.hankel(cf=pc1, t0=1, n=2)
hpc1 <- hankel2cf(hankel=pc1.hankel, id=1)
plot(hpc1, log="y")
heffectivemass1 <- hankel2effectivemass(hankel=pc1.hankel, id=1)</pre>
```

bootstrap.hankel_summed

GEVP method based on Hankel matrices.

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input cf object and a generalised eigenvalue problem is solved then. This is the function to call. It will perform a bootstrap analysis.

Usage

```
bootstrap.hankel_summed(cf, t0values = c(1:(N - 2 * n - deltat)), deltat = 1, n = 2, N = cf$Time/2 + 1)
```

Arguments

| cf | object of type cf |
|----------|---|
| t0values | Integer vector. The t0 values to sum over. Default is c(1:max). All elements must be larger or equal to zero and smaller or equal than max=N-2*n-deltat |
| deltat | Integer. value of deltat used in the hankel GEVP. Default is 1. |
| n | Integer. Size of the Hankel matrices to generate, default is 2. |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix |

Details

```
See vignette(name="hankel", package="hadron")
```

Value

List object of class "hankel.summed". The eigenvalues are stored in a numeric vector t0, the corresonding samples in t. The reference input times t0values is stored as t0values in the returned list. In addition, deltat is stored in the returned list.

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See Also

```
Other hankel: bootstrap.hankel(), bootstrap.pgevm(), bootstrap.truncated.pgevm(), gevp.hankel(),
gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(),
pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()
```

Examples

```
data(correlatormatrix)
correlatormatrix <- bootstrap.cf(correlatormatrix, boot.R=99, boot.l=1, seed=132435)</pre>
t0 <- 4
correlatormatrix.gevp <- bootstrap.gevp(cf=correlatormatrix, t0=t0, element.order=c(1,2,3,4))
pc1 <- gevp2cf(gevp=correlatormatrix.gevp, id=1)</pre>
pc1.hankel <- bootstrap.hankel_summed(cf=pc1, t0=c(1:15), n=2)</pre>
```

bootstrap.lanczos

Lanczos method for LOCD correlators

Description

Taking a single correlation function as input, the method determines the ground state energy plus its bootstrap uncertainty.

Usage

```
bootstrap.lanczos(cf, N = (cf$Time/2 + 1), bias_correction = FALSE,
 errortype = "outlier-removal", pivot = FALSE, probs = c(0.16, 0.84))
```

Arguments

cf object of type cf, optimally returned by bootstrap.cf

Integer. Maximal time index in correlation function to be used in Lanczos anal-N

ysis

bias_correction

boolean. If set to 'TRUE', the median of the bootstrap distribution is used as estimator for the energy values. This will be set to TRUE for errortyp is equal

'dbboot'

string. Determines the treatment of the bootstrap histograms to determine the errortype

> statistical error on eigenvalues. Can be: 1. 'outlier-removal' for which outliers are removed according to the 0.25 and 0.75 quantiles and the inter-quantilerange, i.e. only values are kept which are in the interval $[Q_25 - 1.5IQR, Q_75 +$ 1.5IQR] and the error is computed from the standard deviation of the bootstrap distribution. 2. 'quantiles' for which the error is estimated from the difference between the 0.16 and 0.84 quantile of the original bootstrap distribution 3. 'dbboot' which works only, if the 'cf' is double bootstrapped. It will estimate the

error from the true error of the median

boolean. If set to 'TRUE', the eigenvalues on the original data are used to find pivot

the "correct" eigenvalue on the bootstrap sample by the smallest distance.

numeric. Vector of probabilities for the error estimation method 'quantiles'. probs

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Value

Returns an object of S3 class effectivemass.

References

M. Wagman, 'Lanczos, the transfer matrix, and the signal-to-noise problem', arXiv:2406.20009

See Also

```
plot.effectivemass, bootstrap.effectivemass
Other lanczos: lanczos.solve()
```

Examples

```
data(pscor.sample)
newcf <- cf_orig(cf=t(array(pscor.sample[,2], dim=c(48, 316))))
newcf <- cf_meta(newcf, nrObs=1, Time=48, symmetrised=FALSE)
newcf.boot <- bootstrap.cf(newcf)
ncf.boot <- symmetrise.cf(newcf.boot)
ncf.effmass <- bootstrap.effectivemass(ncf.boot)
plot(ncf.effmass, ylim=c(0.1,0.2))
res <- bootstrap.lanczos(newcf.boot, N=newcf$Time)
plot(res, rep=TRUE, col="red", pch=22, xshift=0.2)</pre>
```

bootstrap.meanerror

Compute the bootstrap error of the mean

Description

Compute the bootstrap error of the mean

Usage

```
bootstrap.meanerror(data, R = 400, l = 20)
```

Arguments

| data | Original data to bootstrap |
|------|---------------------------------|
| R | Number of bootstrap replicates. |
| 1 | Block length. |

Value

Returns a numeric vector with the estimated standard error of the mean.

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bootstrap.nlsfit

Bootstrap a non-linear least-squares fit

Description

Performs and bootstraps a non-linear least-squares fit to data with y and x errors.

Usage

```
bootstrap.nlsfit(fn, par.guess, y, x, bsamples, priors = list(param = c(), p
= c(), psamples = c()), ..., lower = rep(x = -Inf, times =
length(par.guess)), upper = rep(x = +Inf, times = length(par.guess)), dy,
dx, CovMatrix, gr, dfn, mask, use.minpack.lm = TRUE, parallel = FALSE,
error = sd, cov_fn = cov, maxiter = 500, success.infos = 1:3,
relative.weights = FALSE, na.rm = FALSE)
```

Arguments

| fn | fn(par, x,). The (non-linear) function to be fitted to the data. Its first argument must be the fit parameters named par. The second must be x, the explaining variable. Additional parameters might be passed to the function. Currently we pass boot.r which is \emptyset for the original data and the ID $(1,)$ of the bootstrap sample otherwise. As more parameters might be added in the future it is recommended that the fit function accepts as the last parameter to be forward compatible. |
|-----------|--|
| par.guess | initial guess values for the fit parameters. |
| У | the data as a one-dimensional numerical vector to be described by the fit function. |
| x | values of the explaining variable in form of a one-dimensional numerical vector. |
| bsamples | bootstrap samples of y (and x, if applicable). Must be provided as array of dimensions $c(boot.R, n)$ with n equals to length(y) in case of 'yerrors' and For 'xyerrors' to length(y) + length(x). |
| priors | List possessing the elements param, p and psamples. The vector param includes the indices of all fit parameters that are to be constrained and the vector p the corresponding paramater values (e.g. known from a previous fit). The list element psamples is a matrix of dimensions (boot.R, length(param)) and contains the corresponding bootstrap samples. If this list is not specified priors are omitted within the fit. |
| | Additional parameters passed to fn, gr and dfn. |
| lower | Numeric vector of length length(par.guess) of lower bounds on the fit parameters. If missing, -Inf will be set for all. |
| upper | Numeric vector of length length(par.guess) of upper bounds on the fit pa- |

rameters. If missing, +Inf will be set for all.

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dy, dx

Numeric vector. Errors of the dependent and independent variable, respectively.

These do not need to be specified as they can be computed from the bootstrap samples. In the case of parametric bootstrap it might would lead to a loss of information if they were computed from the pseudo-bootstrap samples. They

must not be specified if a covariance matrix is given.

CovMatrix complete variance-covariance matrix of dimensions c(length(y), length(y))

or c(length(y)+length(x),length(y)+length(x)) depending on the errormodel. Pass NULL if the matrix has to be calculated from the bsamples. In that case, if the number of boostrap samples is small compared to the number of variables, singular value decomposition with small eigenvalue replacement will be used (see invertCovMatrix) to attempt a clean inversion. In case a variance-covariance matrix is passed, the inversion will simply be attempted using solve on the Cholesky decomposition. Finally, if CovMatrix is missing, an uncorre-

lated fit will be performed.

gr gr(par, x, ...). gr=d(fn) / d(par) is a function to return the gradient of fn.

It must return an array with length(x) rows and length(par) columns.

dfn dfn(par, x, ...). dfn=d(fn) / dx is the canonical derivative of fn by x and

only relevant if x-errors are provided.

mask logical or integer index vector. The mask is applied to select the observations

from the data that are to be used in the fit. It is applied to x, y, dx, dy, bsamples

and CovMatrix as applicable.

use.minpack.lm use the minpack.lm library if available. This is usually faster than the default

optim but somtimes also less stable.

parallel parallelise over bootstrap samples. The package parallel is required.

error Function that takes a sample vector and returns the error estimate. This is a

parameter in order to support different resampling methods like jackknife.

cov_fn function. Function to compute the covariance (matrix). Default is cov.

maxiter integer. Maximum number of iterations that can be used in the optimization

process.

success.infos integer vector. When using minpack.lm there is the info in the return value.

Values of 1, 2 or 3 are certain success. A value of 4 could either be a success or a saddle point. If you want to interpret this as a success as well just pass 1:4

instead of the default 1:3.

relative.weights

are the errors on y (and x) to be interpreted as relative weights instead of absolute ones? If TRUE, the covariance martix of the fit parameter results is multiplied

by chi^2/dof. This is the default in many fit programs, e.g. gnuplot.

na.rm logical. If set to true, NAs in y and dy will be ignored. If x-errors are taken

into account, NAs in x and dx will be ignored, too.

Value

returns a list of class 'bootstrapfit'. It returns all input parameters and adds in addition the following:

the one dimensional numerical vector of length npar+1. npar is the number of fit parameters. In case of 'yerrors' this equals length(par.guess). For 'xyerrors' this equals length(par.guess) + length(x). to contains the best fit

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parameters obtained on the original data. The last element in t0 is the chisquare value.

t an array of dimensions (npar+1, boot.R) with npar as in t0. The rows contain

the individual bootstrap observations.

bsamples the bootstrap samples used as an array of dimensions (length(y), boot.R) or

(length(y)+length(x), boot.R) depending on the error model with npar as

in t0.

Qval the p-value of the fit on the original data

chisqr the residual chisqr value.

dof the residual degrees of freedom of the fit.

nx the number of x-values.

tofn the original ... list of parameters to be passed on to the fit function

mask original mask value

See Also

Other NLS fit functions: parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()

Examples

```
## Declare some data.
value <- c(0.1, 0.2, 0.31)
dvalue <- c(0.01, 0.01, 0.015)
x \leftarrow c(1, 2, 3)
dx <- c(0.1, 0.1, 0.1)
boot.R <- 1500
fn <- function (par, x, boot.r, ...) par[1] + par[2] * x
## Before we can use the fit with this data, we need to create bootstrap
## samples. We do not want to use the correlation matrix here. Note that you
## can simply use the parametric.nlsfit function as a convenient wrapper of
## the two steps.
bsamples <- parametric.bootstrap(boot.R, c(value, x), c(dvalue, dx))</pre>
head(bsamples)
fit.result <- bootstrap.nlsfit(fn, c(1, 1), value, x, bsamples)</pre>
summary(fit.result)
plot(fit.result, main = 'Ribbon on top')
plot(fit.result, ribbon.on.top = FALSE, main = 'Ribbon below')
residual_plot(fit.result, main = 'Residual Plot')
```

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| ootstrap.pgevm | PGEVM |
|----------------|-------|
| | |

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input cf object and a generalised eigenvalue problem is solved then. This is the function to call. It will perform a bootstrap analysis.

Usage

```
bootstrap.pgevm(cf, deltat = 1, Delta = 1, N = (cf$Time/2 + 1), t0 = 0,
    n.max = floor(((N - 1 - t0 - deltat)/Delta)/2 + 1), submatrix.size = 1,
    element.order = 1, ndep.Delta = FALSE, block.Delta = FALSE,
    custom.indices = NA)
```

Arguments

| cf | object of type cf |
|----------------|---|
| deltat | Integer. value of deltat used in the hankel GEVP. Default is 1. Used t@fixed=FALSE |
| Delta | integer. Delta is the time shift used in the Hankel matrix. |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix |
| t0 | Integer. Initial time value of the GEVP, must be in between 0 and Time/2-n. Default is 1. Used when tofixed=TRUE. |
| n.max | Integer. Maximal Size of the Hankel matrices to generate |
| submatrix.size | Integer. Submatrix size to be used in build of Hankel matrices. Submatrix.size > 1 is experimental. |
| element.order | Integer vector. specifies how to fit the n linearly ordered single correlators into the correlator matrix for submatrix.size > 1. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Matrix elements can occur multiple times, such as c(1,2,2,3) for the symmetric case, for example. |
| ndep.Delta | boolean. If set to 'TRUE', Delta will be chosen 'n' dependent to cover the largest possible range in the correlator. |
| block.Delta | boolean. If set to 'TRUE', the Hankel matrices will be built as connected blocks. Should only be used for symmetric correlators, incompatible with ndep.Delta. |
| custom.indices | integer. Vector of indices to be using in cf instead of computing them from 'Delta' and 't0' |

Details

tbw

Value

List object of class "PGEVM". The eigenvalues are stored in a numeric vector t0, the corresonding samples in t. The reference input time t0 is stored as reference_time in the returned list.

References

Ostmeyer, Sen, Urbach, Eur.Phys.J.A 61 (2025) 2, 26, arXiv:2411.14981, https://doi.org/10.1140/epja/s10050-025-01495-8

See Also

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.truncated.pgevm(), gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

bootstrap.truncated.pgevm

Truncated PGEVM

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input cf object, truncated via SVD and a generalised eigenvalue problem is solved then. This is the function to call. It will perform a bootstrap analysis.

Usage

```
bootstrap.truncated.pgevm(cf, deltat = 1, Delta = 1, N = (cf$Time/2 + 1),
  t0 = 1, n = floor(((N - 1 - t0 - deltat)/Delta)/2 + 1),
  submatrix.size = 1, element.order = 1, max.truncation = n *
  submatrix.size, error.weights = FALSE, symmetric = cf$symmetrised,
  bootstrap.coeffs = FALSE, eps = 1e-15)
```

Arguments

| cf | object of type cf |
|----------------|---|
| deltat | Integer. value of deltat used in the hankel GEVP. Default is 1. Used t0fixed=FALSE |
| Delta | integer. Delta is the time shift used in the Hankel matrix. |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix. |
| t0 | Integer. Initial time value of the GEVP, must be in between 0 and Time/2-n. Default is 1. Used when tofixed=TRUE. |
| n | Integer. Maximal size of the Hankel matrices to generate. Total Hankel matrix dimension will be n*submatrix.size. |
| submatrix.size | Integer. Submatrix size to be used in build of Hankel matrices. |
| element.order | Integer vector. specifies how to fit the n linearly ordered single correlators into the correlator matrix for submatrix.size > 1. E.g. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Matrix elements can occur multiple times, such as c(1,2,2,3) for the symmetric case. |
| max.truncation | Integer. Maximal truncation dimension to be used. Default is n*submatrix.size, the maximal possible value. |

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error.weights boolean or numeric vector. If 'FALSE', no error weighting is applied. If 'TRUE',

the inverse standard error of the correlator is used as weights. If a numeric vector is given, it must be of the same length as cf\$cf0 and contains the weights to

be used.

symmetric boolean. If 'TRUE', the energy spectrum is guaranteed to be symmetric about

0. Default is cf\$symmetrised.

bootstrap.coeffs

boolean. If 'TRUE', the correlator coefficients are also calculated for each boot-

strap sample, not only the original data.

eps numeric. Threshold for the singular value in the SVD to be considered for the

proposed truncation dimension returned as opt.idx. Default is 1e-15.

Details

tbw

Value

List object of classes "PGEVM" and "truncated.pgevm". The eigenvalues are stored in a numeric vector evs, the corresponding samples in evs.tsboot.

See Also

```
Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()
```

c.cf

Concatenate correlation function objects

Description

Concatenate correlation function objects

Usage

```
## S3 method for class 'cf' c(...)
```

Arguments

... Zero or multiple objects of type cf.

Value

Returns an object of class cf representing the concatenation of all the input objects of class cf.

c.raw_cf

Concatenate raw_cf correlation function objects

Description

Concatenate raw_cf correlation function objects

Usage

```
## S3 method for class 'raw_cf'
c(...)
```

Arguments

Zero or multiple objects of type raw_cf.

Value

Returns an object of S3 class raw_cf, the concatenation of the input objects.

```
cA2.09.48_3pi_I3_0_A1u_1_pc
```

A three pion correlator with significant thermal states.

Description

A three pion correlator with significant thermal states.

Usage

```
cA2.09.48_3pi_I3_0_A1u_1_pc
```

Format

An object of class list (inherits from cf, cf_meta, cf_boot, cf_principal_correlator) of length 19.

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cdh

finite size corrections a la Colangelo, Duerr, Haefeli

Description

finite size corrections a la Colangelo, Duerr, Haefeli

Usage

```
cdh(parm = rep(0, times = 6), rev = -1, aLamb1 = 0.055, aLamb2 = 0.58, aLamb3, aLamb4, ampiV, afpiV, aF0, a_fm, L, printit = FALSE, incim6 = FALSE, rtilde = c(-1.5, 3.2, -4.2, -2.5, 3.8, 1), use.cimp1 = TRUE)
```

Arguments

| parm | parameters |
|-----------|--|
| rev | $rev = -1$ corrects from L to $L = \infty$, $rev = +1$ the other way around |
| aLamb1 | The four low energy Λ_{1-4} constants in lattice units. |
| aLamb2 | see aLamb1. |
| aLamb3 | see aLamb1. |
| aLamb4 | see aLamb1. |
| ampiV | pseudo scalar mass values to be corrected |
| afpiV | pseudo scalar decay constant values to be corrected |
| aF0 | af_0 in lattice units |
| a_fm | the value of the lattice spacing in fermi |
| L | the lattice spatial extent |
| printit | if set to TRUE the corrections are printed |
| incim6 | in- or exclude the NNNLO correction for the mass |
| rtilde | the low energy constants \tilde{r} , needed only if incim6=TRUE |
| use.cimpl | use the four times faster direct c Implementation of the correction routine |

Details

see reference for details. We use the simplyfied formulae for the S quantities, see eq. (59) in the reference.

Value

a list with the corrected values for mpi and fpi

Author(s)

Carsten Urbach curbach@gmx.de

36 cdhnew

References

Gilberto Colangelo, Stephan Durr, Christoph Haefeli, Nucl.Phys.B721:136-174,2005. hep-lat/0503014

Examples

cdhnew

finite size corrections a la Colangelo, Duerr, Haefeli, but re-expanded as series in the quark mass

Description

finite size corrections a la Colangelo, Duerr, Haefeli, but re-expanded as series in the quark mass

Usage

```
cdhnew(parm = rep(0, times = 6), rev = -1, aLamb1 = 0.055,
aLamb2 = 0.58, aLamb3, aLamb4, ampiV, afpiV, aF0, a2B0mu, L,
printit = FALSE, use.cimpl = TRUE)
```

Arguments

| parm | m parameters |
|--------|---|
| rev | $rev = -1$ corrects from L to $L = \infty, rev = +1$ the other way around |
| aLamb1 | The four low energy Λ_{1-4} constants in lattice units. |
| aLamb2 | see aLamb1. |
| aLamb3 | see aLamb1. |
| aLamb4 | see aLamb1. |
| ampiV | pseudo scalar mass values to be corrected |
| afpiV | pseudo scalar decay constant values to be corrected |
| aF0 | af_0 in lattice units |
| a2B0mu | $2B_0\mu$ in lattice units, where μ is the quark mass and B_0 a low energy constant |

cdhnew 37

L the lattice spatial extent

printit if set to TRUE the corrections are printed

use.cimpl use the four times faster direct c Implementation of the correction routine

Details

see reference for details. We use the simplyfied formulae for the S quantities, see eq. (59) in first reference.

Value

a list with the corrected values for mpi and fpi

Author(s)

Carsten Urbach curbach@gmx.de

References

Gilberto Colangelo, Stephan Durr, Christoph Haefeli, Nucl.Phys.B721:136-174,2005. hep-lat/0503014 and

R. Frezzotti, V. Lubicz, S. Simula, arXiv:0812.4042 hep-lat

```
mu < -c(0.004, 0.006, 0.008, 0.010, 0.004)
L <- c(24, 24, 24, 24, 32)
mps <- c(0.14448, 0.17261, 0.19858, 0.22276, 0.14320)
fps <- c(0.06577, 0.07169, 0.07623, 0.07924, 0.06730)
aLamb1 <- 0.05
aLamb2 <- 0.5
aLamb3 <- 0.38
aLamb4 <- 0.66
aF0
      <- 0.051
       <- 5.64
a2B
cdhres <- cdhnew(rev=+1, aLamb1=aLamb1, aLamb2=aLamb2, aLamb3=aLamb3,</pre>
                 aLamb4=aLamb4, ampiV=mps, afpiV=fps, aF0=aF0,
                 a2B0mu=a2B*mu, L=L, printit=TRUE)
cdhres$mpiFV
cdhres$fpiFV
```

38 CExp

CExp

Cosh Or Sinh Build Out Of Two Exps

Description

Evaluates

$$f(x) = \frac{1}{2}(\exp(-m(T-x)) \pm \exp(-mx))$$

for given mass m, vector x and time extent T. This form is better usable in χ^2 fitting than cosh or sinh.

Usage

```
CExp(m, Time, x, sign = 1)
```

Arguments

m mass valueTime Time extent

x vector of values on which to evaluate the function

sign with sign=1 cosh is evaluated, with sign=-1 sinh

Value

```
vector f(x)
```

Author(s)

Carsten Urbach <carsten.urbach@liverpool.ac.uk>

```
m <- 0.1
Time <- 48
x <- seq(0, 48, 1)
CExp(m=m, Time=Time, x=x)</pre>
```

cf

cf

Correlation function container

Description

This function cf() creates containers for correlation functions of class cf. This class is particularly designed to deal with correlation functions emerging in statistical and quantum field theory simulations. Arithmetic operations are defined for this class in several ways, as well as concatenation and is.cf.

Usage

cf()

Details

And last but not least, these are the fields that are used somewhere in the library but we have not figured out which mixin these should belong to:

• conf.index: TODO

• N: Integer, number of measurements.

• blockind: TODO

• jack.boot.se: TODO

Value

returns an object of S3 class cf derived from a list

See Also

```
Other cf constructors: cf_boot(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_subtracted(), cf_weighted()
```

```
newcf <- cf()</pre>
```

40 cf_boot

| cf_boot | Bootstrapped CF mixin constructor | |
|---------|-----------------------------------|--|
| | | |

Description

Bootstrapped CF mixin constructor

Usage

```
cf_boot(.cf = cf(), boot.R, boot.l, seed, sim, endcorr, cf.tsboot,
  icf.tsboot = NULL, resampling_method)
```

Arguments

| .cf | cf object to extend. |
|-----------------|--|
| boot.R | Integer, number of bootstrap samples used. |
| boot.1 | Integer, block length in the time-series bootstrap process. |
| seed | Integer, random number generator seed used in bootstrap. |
| sim | Character, sim argument of tsboot. |
| endcorr | Boolean, endcorr argumetn of tsboot. |
| cf.tsboot | List, result from the tsboot function for the real part. |
| icf.tsboot | List, result from the tsboot function for the imaginay part. |
| resampling_meth | nod |
| | Character, either 'bootstrap' or 'jackknife' |

Details

The following fields will also be made available:

- cf0: Numeric vector, mean value of original measurements, convenience copy of cf. tsboot\$t0.
- tsboot.se: Numeric vector, standard deviation over bootstrap samples.
- boot.samples: Logical, indicating whether there are bootstrap samples available. This is deprecated and instead the presence of bootstrap samples should be queried with inherits(cf, 'cf_boot').
- error_fn: Function, takes a vector of samples and computes the error. In the bootstrap case this is just the sd function. Use this function instead of a sd in order to make the code compatible with jackknife samples.

Value

returns the input object of class cf with the bootstrap mixin added

See Also

```
Other cf constructors: cf(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_subtracted(), cf_weighted()
```

cf_key_meson_2pt 41

| cf_key_meson_2pt Generate key string to identify a meson 2pt function | |
|---|--|
|---|--|

Description

Generate key string to identify a meson 2pt function

Usage

```
cf_key_meson_2pt(fwd_flav, bwd_flav, snk_gamma, src_gamma, src_p, snk_p)
```

Arguments

| fwd_flav | String, "forward" quark flavour identifier. |
|-----------|--|
| bwd_flav | String, "backward" quark flavour identifier. |
| snk_gamma | Integer, CVC convention gamma matrix identifier at the source. |
| src_gamma | Integer, CVC convention gamma matrix identified at the sink. |
| src_p | Integer vector of length 3. (x,y,z) components of the source momentum vector in lattice units. |
| snk_p | Integer vector of length 3. (x,y,z) components of the sink momentum vector in lattice units. |

Value

A character vector with the HDF5 key.

| cf_key_meson_3pt | Generate HDF5 key for CVC 'correlators' meson 3pt function with a local or derivative insertion |
|------------------|---|
| | |

Description

The key for a meson three-point function has the form:

```
/sud+-g-u-g/t10/dt12/gf5/pfx0pfy0pfz0/gc0/Ddim0_dir0/Ddim1_dir1/D[...]/gi5/pix0piy0piz0 where, from left to right: * 'u' is the flavour of the "backward" propagator * 'd' is the flavour of the "sequential" propagator * '+' indicates that 'sud' is daggered * 'g' indicates a gamma insertion * 'u' is the flavour of the foward propagator * 'g' indicates a Dirac structure at the source * 'tXX' is the source time slice * 'dtYY' is the source-sink separation * 'gfN' gamma structure at the sink in CVC indexing * 'pfxXpfyYpfzZ' is the sink momentum in CVC convention (sink and source phases are both exp(ipx)) * 'gcN' gamma structure at the current insertion point in CVC indexing * 'DdimJ_dirK' covariant displacement applied in dimension 'J', direction 'K' where it should be noted that this is. in operator notation, i.e., the right-most displacement is the one applied first. * [...] * 'giN' gamma structure at the source in CVC indexing * 'pixXpiyYpizZ' at the source in CVC convention
```

42 cf_meta

Usage

```
cf_key_meson_3pt(fwd_flav, bwd_flav, seq_flav, dt, snk_gamma, cur_gamma,
    cur_displ_dim = NA, cur_displ_dir = NA, src_gamma, src_p, snk_p)
```

Arguments

| fwd_flav | String, "forward" quark flavour identifier. |
|---------------|--|
| bwd_flav | String, "backward" quark flavour identifier. |
| seq_flav | String, "sequential" quark flavour identifier. |
| dt | Integer, source-sink separation. |
| snk_gamma | Integer, CVC convention gamma matrix identifier at the source. |
| cur_gamma | Integer, CVC convention gamma matrix identified at the insertion. |
| cur_displ_dim | Integer vector of dimensions $(0,1,2,3 <-> t,x,y,z)$ in which covariant displacements have been applied. This vector will be parsed in reverse order, such that the first element here is the first displacement applied to the spinor in the calculation and the right-most element in the key. Length must be matched to 'cur_displ_dir'. Defaults to 'NA' for no displacements. |
| cur_displ_dir | Integer vector of directions (forward, backward) $<->$ (0,1) in which the covariant displacements have been applied. Parsing as for 'cur_displ_dim'. Length must be matched to 'cur_displ_dim'. Defaults to 'NA' for no displacements. |
| src_gamma | Integer, CVC convention gamma matrix identified at the sink. |
| src_p | Integer vector of length 3. (x,y,z) components of the source momentum vector in lattice units. |
| snk_p | Integer vector of length 3. (x,y,z) components of the sink momentum vector in lattice units. |

Value

A character vector with the HDF5 key.

Description

CF metadata mixin constructor

```
cf_meta(.cf = cf(), nrObs = 1, Time = NA, nrStypes = 1,
    symmetrised = FALSE)
```

cf_orig 43

Arguments

.cf cf object to extend.

nr0bs Integer, number of different measurements contained in this correlation func-

tion. One can use c.cf to add multiple observables into one container. This is for

instance needed when passing to the gevp function.

Time Integer, full time extent.

nrStypes Integer, number of smearing types.

symmetrised Logical, indicating whether the correlation function has been symmetrized.

Value

returns the input object of class cf with the metadata mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_subtracted(), cf_weighted()
```

Examples

```
newcf <- cf_orig(cf=array(rnorm(25*100), dim=c(100, 25)))
newcf <- cf_meta(newcf, nr0bs=1, Time=48, symmetrised=TRUE)</pre>
```

cf_orig

Original data CF mixin constructor

Description

Original data CF mixin constructor

Usage

```
cf_orig(.cf = cf(), cf, icf = NULL)
```

Arguments

| .cf | cf object to extend. Named with a leading period just to distinguish it from the |
|-----|--|
| | member also named cf. |
| - £ | Numeric metalic spinished data for all absorbed and measurements |

cf Numeric matrix, original data for all observables and measurements.

Numeric matrix, imaginary part of original data. Be very careful with this as quite a few functions just ignore the imaginary part and drop it in operations.

Value

icf

returns the input object of class cf with the original data mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_subtracted(), cf_weighted()
```

Examples

```
newcf <- cf_orig(cf=array(rnorm(25*100), dim=c(100, 25)))
newcf <- cf_meta(newcf, nrObs=1, Time=48, symmetrised=TRUE)
newcf <- bootstrap.cf(newcf)
plot(newcf)</pre>
```

```
cf_principal_correlator
```

Principal correlator CF mixin constructor

Description

Principal correlator CF mixin constructor

Usage

```
cf_principal_correlator(.cf = cf(), id, gevp_reference_time)
```

Arguments

Integer, reference time t_0 that has been used in the GEVP.

Value

returns the input object of class cf with the principal correlator mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_orig(), cf_shifted(), cf_smeared(), cf_subtracted(), cf_weighted()
```

cf_shifted 45

| cf | sh | i f | ted |
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Shifted CF mixin constructor

Description

Shifted CF mixin constructor

Usage

```
cf_shifted(.cf = cf(), deltat, forwardshift)
```

Arguments

.cf cf object to extend.

deltat TODO

forwardshift Logical, TODO

Details

The following fields will also be made available:

• shifted: Logical, whether the correlation function has been shifted This is deprecated and instead the presence of a shift should be queried with inherits(cf, 'cf_shifted').

Value

returns the input object of class cf with the shifted mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_smeared(), cf_subtracted(), cf_weighted()
```

cf_smeared

Smeared CF mixin constructor

Description

Smeared CF mixin constructor

```
cf_smeared(.cf = cf(), scf, iscf = NULL, nrSamples, obs)
```

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Arguments

| .cf | cf object to extend. |
|-----------|--------------------------------------|
| scf | Like cf, but with the smeared data. |
| iscf | Like icf, but with the smeared data. |
| nrSamples | TODO |
| obs | TODO |

Details

The following fields will also be made available:

• smeared: Logical, whether the correlation function has smeared data. This is deprecated and instead the presence of bootstrap samples should be queried with inherits(cf, 'cf_smeared').

Value

returns the input object of class cf with the smeared mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_subtracted(), cf_weighted()
```

cf_subtracted

Subtracted CF mixin constructor

Description

Subtracted CF mixin constructor

Usage

```
cf_subtracted(.cf = cf(), subtracted.values, subtracted.ii)
```

Arguments

```
.cf cf object to extend.
subtracted.values
Numeric matrix, TODO
subtracted.ii Integer vector, TODO
```

Value

returns the input object of class cf with the subtracted mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_weighted()
```

cf_weighted 47

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|-----|--------|------|
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| CI_ | _weigh | teu |

Weighted CF mixin constructor

Description

Weighted CF mixin constructor

Usage

```
cf_weighted(.cf = cf(), weight.factor, weight.cosh)
```

Arguments

```
.cf cf object to extend.
weight.factor TODO
weight.cosh TODO
```

Details

The following fields will also be made available:

• weighted: Logical, indicating whether the correlation function has been weighted. This is deprecated and instead the presence of this should be queried with inherits(cf, 'cf_weighted').

Value

returns the input object of class cf with the weighted mixin added

See Also

```
Other cf constructors: cf(), cf_boot(), cf_meta(), cf_orig(), cf_principal_correlator(), cf_shifted(), cf_smeared(), cf_subtracted()
```

compute.plotlims

compute.plotlims

Description

Computes limits for plots

```
compute.plotlims(val, logscale, cumul.dval, cumul.mdval)
```

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Arguments

val Numeric. Value.

logscale Boolean.

cumul.dval Numeric. Cumulative error. cumul.mdval Numeric. Cumulative error.

Value

The computed plot limits are returned as a two component numeric vector.

computeacf Computes The ACF and Integrated AC Time

Description

Computes the ACF and integrated autocorrelation time of a time series. It also estimates the corresponding standard errors.

Usage

```
computeacf(tseries, W.max, Lambda = 100)
```

Arguments

tseries the time series.

W.max maximal time lag to be used.

Lambda cut-off needed to estimate the standard error of the ACF.

Details

The standard error of the ACF is computed using equation (E.11) of M. Luescher, hep-lat/0409106. The error of the integrated autocorrelation time using the Madras Sokal formula, see also hep-lat/0409106.

Value

It returns a list of class hadronacf with members

lags time lags of the integrated autocorrelation function

Gamma normalised autocorrelation function

dGamma error of normalised autocorrelation function

W.max max time lag used for the call of acf

W the cut-off up to which the ACF is integrated for the integrated autocorrelation

time

tdata the original time series

tau the estimated integrated autocorrelation time

dtau the estimated error of the integrated autocorrelation time

computeDisc 49

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

'Monte Carlo errors with less errors', Ulli Wolff, http://arxiv.org/abs/hep-lat/0306017hep-lat/0306017

'Schwarz-preconditioned HMC algorithm for two-flavour lattice QCD', Martin Luescher, http://arxiv.org/abs/hep-lat/0409106

N. Madras, A. D. Sokal, J. Stat. Phys. 50 (1988) 109

See Also

```
uwerr, acf bootstrap.analysis
```

Examples

```
data(plaq.sample)
myacf <- computeacf(plaq.sample, 300)
plot(myacf)
summary(myacf)</pre>
```

computeDisc

computes a disconnected correlation function from loops

Description

The dimension of cf\$cf and cf\$icf must be dim(Time, S, N), where Time is the time extent, S is the number of samples and N the number of measurements (gauges). cf2 is the same, but needed only for cross-correlators.

Usage

```
computeDisc(cf, cf2, real = TRUE, real2 = TRUE, smeared = FALSE,
  smeared2 = FALSE, subtract.vev = TRUE, subtract.vev2 = TRUE,
  subtract.equal = TRUE, use.samples, use.samples2, type = "cosh",
  verbose = FALSE)
```

Arguments

| cf | loop data as produced by readcmidisc or readbinarydisc. |
|---------|--|
| cf2 | second set of loop data as produced by readcmidisc or readbinarydisc. This is needed for cross-correlators |
| real | use the real part cf\$cf, if set to TRUE, otherwise the imaginary part cf\$icf. |
| real2 | use the real part cf2\$cf, if set to TRUE, otherwise the imaginary part cf2\$icf. |
| smeared | use the loops instead of the local ones for cf. |

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| smeared2 | use the loops instead of the local ones for cf2. |
|----------------|---|
| subtract.vev | subtract a vacuum expectation value. It will be estimated as mean over all samples, gauges and times available. |
| subtract.vev2 | subtract a vacuum expectation value for the second set of loops. It will be estimated as mean over all samples, gauges and times available. |
| subtract.equal | subtract contributions of products computed on identical samples. This will introduce a bias, if set to FALSE for missing cf2 or if cf and cf2 are computed on the same set of random sources. |
| use.samples | If set to an integer, only the specified number of samples will be used for cf, instead of all samples. |
| use.samples2 | Same like use.samples, but for cf2. |
| type | The correlation function can either be symmetric or anti-symmetric in time. Anti-symmetric is of course only possible for cross-correlators. In this case with type="cosh" it is assumed to be symmetric, anti-symmetric otherwise. |
| verbose | Print some debug output, like the VEVs of the loops. |

Details

If subtract.vev=TRUE the vev is estimated as the mean over all gauges, samples and times available and subtracted from the original loop data. (Same for subtrac.vev2.

The correlation is computed such as to avoid correlation between equal samples, unless nrSamples is equal to 1.

cf and cf2 must agree in Time, number of gauges and number of samples. Matching of gauges is assumed. If this is not the case results are wrong.

Value

Returns an object of type cf derived from a list with elements cf, an array of dimension dim(N, Time), where N is the number of samples and Time the time extent, integers Time for the time extent, nrStypes and nrObs for the available smearing types and operators, and finally nrSamples, the number of samples used to generate the correlation function cf.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readcmidisc, readbinarydisc, bootstrap.cf, add.cf, c.cf
```

```
data(loopdata)
Cpi0v4 <- computeDisc(cf=loopdata, real=TRUE, subtract.vev=TRUE)
Cpi0v4 <- bootstrap.cf(Cpi0v4, boot.R=99, boot.l=1, seed=14556)</pre>
```

computefps 51

| computefps | Computes the pseudoscalar decay constant for the twisted mass case from the pseudoscalar amplitude and mass |
|------------|---|
| | |

Description

From a mass and amplitude determination (using matrixfit or fit.effectivemass, bootstrap.gevp and gevp2amplitude the pseudoscalar decay constant is determined for the case of Wilson twisted mass fermions from the pseudoscalar amplitude and mass

Usage

```
computefps(mfit, PP, mass, mu1, mu2, Kappa, normalisation = "cmi",
    disprel = "continuum", boot.fit = TRUE)
```

Arguments

| mfit | An object of type matrixfit or gevp.amplitude generated with matrixfit or gevp2amplitude, respectively. |
|--------------------------|---|
| PP | If mfit is missing this must contain the value for the pseudoscalar amplitude. |
| mass | If mfit is missing this must contain the value for the pseudoscalar mass. |
| mu1, mu2 | The values for the twisted quark masses involved in the pseudoscalar meson. If mu2 is missing it will be assumed to be equal to mu1. |
| Карра | The κ -value of the run, needed only if normalisation="cmi". |
| | |
| normalisation | normalisation of the correlators. If set to "cmi" the κ value must be specified. |
| normalisation disprel | normalisation of the correlators. If set to "cmi" the κ value must be specified. One of "continuum" or "lattice". Indicates whether the formula for the decay constant should take into account the lattice dispersion relation for the meson. Theoretically this can reduce lattice artefacts for heavy mesons. |

Details

The pseudoscalar decay constant is computed from

$$f_{\rm PS} = 2\kappa(\mu_1 + \mu_2) \frac{PP}{\sqrt{2}\sqrt{m_{\rm PS}}^3}$$

for normalisation="cmi" or

$$f_{\rm PS} = (\mu_1 + \mu_2) \frac{PP}{\sqrt{2}\sqrt{m_{\rm PS}}^3}$$

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expecting physical normalisation of the amplitudes. When disprel="lattice",

$$\sqrt{m_{\rm PS}^3}$$

is replaced with

$$\sqrt{m_{\rm PS}} \sinh m_{\rm PS}$$

which can reduce lattice artefacts for heavy meson masses.

Value

If mfit ist missing the value of fps will printed to stdout and returned as a simple numerical value.

If mfit is available, this object will be returned but with additional objects added: fps, fps.tsboot, mu1, mu2, normalistaion and Kappa if applicable.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
matrixfit, gevp2amplitude,
```

Examples

computefpsOS

Computes the pseudoscalar decay constant for the Osterwalder Seiler case from the pseudoscalar amplitude and mass

Description

From a mass and amplitude determination (using matrixfit) the pseudoscalar decay constant is determined for the case of Osterwalder Seiler (OS) fermions from the AS and SS amplitude (in the twisted basis), ZA and the OS pion mass.

```
computefpsOS(mfit, Kappa = sqrt(0.5), normalisation = "cmi",
boot.fit = TRUE, ZA = 1, ZAboot, dZA)
```

computefpsOS 53

Arguments

mfit An object of type matrixfit generated with matrixfit. The correlation matrix

(SS, SA, AS, AA) must have been analysed, where the correlators are in the

twisted basis.

Kappa The κ -value of the run, needed only if normalisation="cmi".

normalisation normalisation of the correlators. If set to "cmi" the κ value must be specified.

boot.fit If set to FALSE, the computation is not bootstrapped, even if the matrixfit or

gevp.amplitude contain bootstrap samples. This is a useful time-saver if error information is not strictly necessary. Of course, this affects the return values

related to the bootstrap, which are set to NA.

ZA The value of the renormalisation constant Z_A .

ZAboot Bootstrap samples for Z_A . If they are provided, they are used for computing fps,

if not, bootstrap samples are generated from dZA. If both are missing, the error

of Z_A is not taken into account.

dZA The value of the (normally distributed) error of the renormalisation constant Z_A .

Details

The pseudoscalar decay constant is computed from

$$f_{\rm PS}^{\rm OS} = Z_A \sqrt{2} \kappa \frac{\langle 0|A|\pi \rangle}{m_{\rm PS}}$$

for normalisation="cmi" or

$$f_{\mathrm{PS}}^{\mathrm{OS}} = Z_A \frac{\langle 0|A|\pi\rangle}{m_{\mathrm{PS}}}$$

expecting physical normalisation of the amplitudes.

Value

If mfit is available, this object will be returned but with additional objects added: fpsOS, fpsOS.tsboot, normalistaion, ZA, ZAboot and kappa if applicable.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

matrixfit

54 concat.raw_cf

concat.cf

Concatenate two correlation function objects

Description

Concatenate two correlation function objects

Usage

```
concat.cf(left, right)
```

Arguments

left, right cf objects to concatenate.

Value

Returns an object of class cf representing the concatenation of the two input objects of class cf.

concat.raw_cf

Concatenate two raw_cf correlation function objects

Description

The data of the left and right objects is concatenated along the second array dimension such that the output contains the tensor slices of right after the slices of left

Usage

```
concat.raw_cf(left, right)
```

Arguments

left raw_cf object to be concatenated with right right raw_cf object to be concatenated with left

Value

Returns an object of S3 class raw_cf, the concatenation of the two input objects.

conj_raw_cf 55

| conj_raw_cf | Take the complex conjugate of a raw_cf object |
|-------------|---|
| coj ac. | Take the complex confugate of a range rospect |

Description

Take the complex conjugate of a raw_cf object

Usage

```
conj_raw_cf(cf)
```

Arguments

cf raw_cf cotnainer with data

Value

raw_cf

```
construct_onlinemeas_rundir
```

Construct a run directory string for analysis_online

Description

Construct a run directory string for analysis_online

Usage

```
construct_onlinemeas_rundir(type, beta, L, Time, kappa = 0, mul = 0,
  csw = 0, musigma = 0, mudelta = 0, muh = 0, addon = "",
  debug = FALSE)
```

Arguments

| type | String. Short identifier for gauge action type. For example, iwa for Iwasaki gauge action. |
|---------|--|
| beta | Numeric. Inverse gauge coupling. |
| L | Integer. Spatial lattice extent. |
| Time | Integer. Temporal lattice extent. |
| kappa | Numeric. Sea quark action hopping parameter. |
| mul | Numeric. Sea light quark twisted mass. |
| CSW | Numeric. Sea quark action clover parameter. |
| musigma | Numeric. Sea 1+1 "heavy" average twisted quark mass. |

mudelta Numeric. Sea 1+1 "heavy" splitting twisted quark mass.

muh Numeric. In case of n_f=2+2 run, "heavy" twisted quark mass.

addon String. Arbitratry string which will be suffixed to the constructed run directory.

debug Boolean. If TRUE, the constructed directory name is printed to screen.

Value

String. Directory name constructed out of the various function parameters. See source code for details.

correlatormatrix

Sample correlator matrix

Description

Sample data for a correlation function for a 24 cube times 48 lattice QCD simulation representing a pion propagation. It is stored in form of an object of class cf, which is derived from list.

Format

```
list of 7 elements: "nrObs" "Time" "nrStypes" "symmetrised" "cf" "icf" "cf0"
```

Examples

```
data("correlatormatrix")
```

correlators_key_meson_2pt

Generate HDF5 key for CVC 'correlators' meson 2pt function

Description

Generate HDF5 key for CVC 'correlators' meson 2pt function

```
correlators_key_meson_2pt(fwd_flav, bwd_flav, src_ts, snk_gamma, src_gamma,
    src_p, snk_p)
```

Arguments

| fwd_flav | String, "forward" quark flavour identifier. |
|-----------|--|
| bwd_flav | String, "backward" quark flavour identifier. |
| src_ts | Integer, source time slice. |
| snk_gamma | Integer, CVC convention gamma matrix identifier at the source. |
| src_gamma | Integer, CVC convention gamma matrix identified at the sink. |
| src_p | Integer vector of length 3. (x,y,z) components of the source momentum vector in lattice units. |
| snk_p | Integer vector of length 3. (x,y,z) components of the sink momentum vector in lattice units. |

Value

A character vector with the HDF5 key.

```
correlators_key_meson_3pt
```

Generate HDF5 key for CVC 'correlators' meson 3pt function with a local or derivative insertion

Description

The key for a meson three-point function has the form:

```
/sud+-g-u-g/t10/dt12/gf5/pfx0pfy0pfz0/gc0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0piz0/Ddim0\_dir0/Ddim1\_dir1/D[...]/gi5/pix0piy0pix0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddim0_dir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddir0/Ddi
```

where, from left to right: * 'u' is the flavour of the "backward" propagator * 'd' is the flavour of the "sequential" propagator * '+' indicates that 'sud' is daggered * 'g' indicates a gamma insertion * 'u' is the flavour of the foward propagator * 'g' indicates a Dirac structure at the source * 'tXX' is the source time slice * 'dtYY' is the source-sink separation * 'gfN' gamma structure at the sink in CVC indexing * 'pfxXpfyYpfzZ' is the sink momentum in CVC convention (sink and source phases are both exp(ipx)) * 'gcN' gamma structure at the current insertion point in CVC indexing * 'DdimJ_dirK' covariant displacement applied in dimension 'J', direction 'K' where it should be noted that this is. in operator notation, i.e., the right-most displacement is the one applied first. * [...] * 'giN' gamma structure at the source in CVC indexing * 'pixXpiyYpizZ' at the source in CVC convention

```
correlators_key_meson_3pt(fwd_flav, bwd_flav, seq_flav, src_ts, dt, snk_gamma,
  cur_gamma, cur_displ_dim = NA, cur_displ_dir = NA, src_gamma, src_p,
  snk_p)
```

58 create_displ_chains

Arguments

| fwd_flav | String, "forward" quark flavour identifier. |
|---------------|--|
| bwd_flav | String, "backward" quark flavour identifier. |
| seq_flav | String, "sequential" quark flavour identifier. |
| src_ts | Integer, source time slice. |
| dt | Integer, source-sink separation. |
| snk_gamma | Integer, CVC convention gamma matrix identifier at the source. |
| cur_gamma | Integer, CVC convention gamma matrix identified at the insertion. |
| cur_displ_dim | Integer vector of dimensions $(0,1,2,3 <-> t,x,y,z)$ in which covariant displacements have been applied. This vector will be parsed in reverse order, such that the first element here is the first displacement applied to the spinor in the calculation and the right-most element in the key. Length must be matched to 'cur_displ_dir'. Defaults to 'NA' for no displacements. |
| cur_displ_dir | Integer vector of directions (forward, backward) <-> $(0,1)$ in which the covariant displacements have been applied. Parsing as for 'cur_displ_dim'. Length must be matched to 'cur_displ_dim'. Defaults to 'NA' for no displacements. |
| src_gamma | Integer, CVC convention gamma matrix identified at the sink. |
| src_p | Integer vector of length 3. (x,y,z) components of the source momentum vector in lattice units. |
| snk_p | Integer vector of length 3. (x,y,z) components of the sink momentum vector in lattice units. |

Value

A character vector with the HDF5 key.

| create list of chains of displacements Multilpe covariant displacements, when applied in order, form a list of displacments. Each consists of a direction and a dimension. |
|--|
| sists of a direction and a dimension. |
| |

Description

create list of chains of displacements Multilpe covariant displacements, when applied in order, form a list of displacements. Each consists of a direction and a dimension.

```
create_displ_chains(max_depth, dims = c(0:3), dirs = c(0, 1))
```

cvc_local_loop_key 59

Arguments

max_depth Positive integer, number of displacement combinations to construct.

dims Integer vector, which lattice dimensions to consider. Default 0:3

dirs Integer vector, which displacement directions to consider. Default forward and

backward <-> c(0,1)

Value

List of data frames, each with columns 'dim' and 'dir' of 'max_depth' rows.

cvc_local_loop_key

Generate HDF5 key for a momentum and spin-projected CVC loop

Description

Generate HDF5 key for a momentum and spin-projected CVC loop Generate key to identify a momentum and spin-projected loop

Usage

```
cvc_local_loop_key(loop_type, istoch, gamma, p)
cvc_local_loop_key(loop_type, istoch, gamma, p)
```

Arguments

loop_type String, loop type.

istoch Integer, index of the stochastic sample.

gamma Integer, CVC convention gamma matrix identifier.

p Integer vector of length 3, (x,y,z) components of the momentum vector in lattice

units.

Value

A character vector with the HDF5 key.

A character vector with the HDF5 key.

60 cvc_read_loops

cvc_read_loops

read HDF5 loop files in the CVC loop format

Description

The CVC naive_loops code produces HDF5 files which contain a matrix of momenta and the data for the loops (without spin projection) organised by stochastic sample. Currently, the reading code assumes that there is a single configuration stored per file and the "trajectory" parameter in CalcLoops is assumed to take its default value of '4'.

Usage

```
cvc_read_loops(selections, files, Time, nstoch, verbose = FALSE,
    check_group_names = FALSE)
```

Arguments

selections

Named list with names from the list 'Naive', 'Scalar', 'dOp', 'Loops' 'LpsDw', 'LpsDwCv', 'LoopsCv' specifying the requested loop types. The elements of this list are in turn expected be data frames of the form

| qx | $\mathbf{q}\mathbf{y}$ | qz |
|----|------------------------|----|
| 0 | 0 | 1 |
| -2 | 1 | -3 |
| | | |

specifying the momentum combinations to be extracted for each loop type.

files Vector of strings, list of HDF5 files to be processed.

Time Integer, time extent of the lattice.

nstoch Integer, number of stochastic samples to be expected in file.

verbose Boolean, output I/O time per file. Requires 'tictoc' package. Default FALSE.

check_group_names

Boolean, check if the group names that we're about to read actually exist in the file. This is quite slow because it uses rhdf5::h51s. Default FALSE.

Value

Named nested list of the same length as selections containg the loop data in the raw_cf format. Each named element corresponds to one loop type and each element of the underlying numbered list corresponds to one momentum combination as specified via selections for this loop type in the same order.

cvc_to_raw_cf 61

| cvc_to_raw_cf | _ | 'onvert correlation function read from CVC HDF5 or AFF format to 'aw_cf' | |
|---------------|---|--|--|
| | | | |

Description

Given a numeric vector of alternating real and imaginary parts of a correlation function, creates an object of class 'raw_cf' with a single measurement, inferring Time from the passed numeric vector while the shape of the internal dimensions has to be specified explicitly if larger than one by one (c(1,1)).

Usage

```
cvc_to_raw_cf(cf_dat, dims = c(1, 1))
```

Arguments

cf_dat Numeric vector of alternating real and imaginary parts of a correlation function.

Ordering of the input should be complex, internal dimensions, time (left to right,

fastest to slowest).

dims Integer vector with the sizes of the internal dimensions. For example, c(4,4)

for spin correlators.

Value

raw_cf object with a data member which contains the data (as complex numbers) in the shape c(1,nts,dims), where nts is the number of time slices inferred from the length of cfdat and the product of the internal dimensions dims.

```
cyprus_make_key_scalar
```

HDF5 key for Cyprus CalcLoops scalar-type loops

Description

Generates an HDF5 key (full path) for the scalar type loops from the Cyprus CalcLoops application.

```
cyprus_make_key_scalar(istoch, loop_type, cid = 4, accumulated = FALSE)
```

Arguments

| istoch | Integer, index of the stochastic sample that the key should be generated for. |
|--------|---|
| | |

loop_type String, name of loop type. Allowed values: 'Scalar', 'dOp'

cid Integer, configuration number, internally produced by the CalcLoops tool via

the "trajectory" input flag. The default is '4' as this is often not used in practice.

accumulated Boolean, depending on whether the loop data was accumulated over the stochas-

tic source d.o.f. or not, the keys are different. Default: FALSE

Value

A character vector with the HDF5 key.

cyprus_make_key_vector

HDF5 key for Cyprus CalcLoops derivative-type loops

Description

Generates an HDF5 key (full path) for the derivative type loops from the Cyprus CalcLoops application.

Usage

```
cyprus_make_key_vector(istoch, loop_type, dir, cid = 4,
   accumulated = FALSE)
```

Arguments

| istoch | Integer, index of the stochastic sample that the key should be generated for. |
|-------------|---|
| loop_type | String, name of loop type. Allowed values: 'Loops', 'LpsDw', 'LpsDwCv', 'LoopsCv' |
| dir | Integer, lattice direction of the derivative. Allowed values: $0 == x$, $1 == y$, $2 == z$, $3 == t$. |
| cid | Integer, configuration number, internally produced by the CalcLoops tool via the "trajectory" input flag. The default is '4' as this is often not used in practice. |
| accumulated | Boolean, depending on whether the loop data was accumulated over the stochas- |

tic source d.o.f. or not, the keys are different. Default: FALSE

Value

A character vector with the HDF5 key.

cyprus_read_loops 63

cyprus_read_loops

read HDF5 loop files in the Cyprus CalcLoops format

Description

The CalcLoops code produces HDF5 files which contain a matrix of momenta and the data for the loops (without spin projection) organised by stochastic sample. Currently, the reading code assumes that there is a single configuration stored per file.

Usage

```
cyprus_read_loops(selections, files, Time, nstoch, accumulated = TRUE,
  legacy_traj = TRUE, verbose = FALSE, check_group_names = FALSE,
  spin_project = FALSE, project_gamma = NULL, use_parallel = TRUE)
```

Arguments

selections

Named list with names from the list 'Naive', 'Scalar', 'dOp', 'Loops' 'LpsDw', 'LpsDwCv', 'LoopsCv' specifying the requested loop types. The elements of this list are in turn expected be data frames of the form

| рx | рy | pz |
|----|----|----|
| 0 | 0 | 1 |
| -2 | 1 | -3 |
| | | |

specifying the momentum combinations to be extracted for each loop type.

files Vector of strings, list of HDF5 files to be processed.

Time Integer, time extent of the lattice.

nstoch Integer, number of stochastic samples to be expected in file.

accumulated Boolean or vector of boolean, specifies whether the loops, as organised by

stochastic sample, are accumulated, such that, say, element n corresponds to the sum over the first n stochastic samples. If specified as TRUE, the data is post-processed to recover the measurements for the particular samples. In case this is specified as a vector, it must be of the same length as files. Default: TRUE.

legacy_traj Boolean. The root group for the loop data is 'conf_xxxx', where 'xxxx' corre-

sponds to what is passed via the 'traj' flag to CalcLoops. When left empty, this defaults to '0004'. If this was left emtpy when the loop files were generated, set this to TRUE and the paths will be constructed with 'conf_0004' as their root group. When specified as a vector, it must be of length length(files) giving

the integer configuration indices, such as c(0, 2, 4, 6) Default: TRUE.

verbose Boolean, output I/O time per file. Requires 'tictoc' package. Default FALSE.

check_group_names

Boolean, employ rhdf5::h51s to check if all the group names that we want to read are actually in the file. This can be slow for large files. Default: FALSE.

disc_3pt

spin_project
Boolean, whether the loops should be spin projected after being read. Must be provided to together with project_gamma! Default: FALSE

project_gamma
Named list of the same length as selections containing, for each selected loop type a 4x4 complex-valued projection matrix. For vector loop types, one matrix must be provided per direction (so project_gamma\$loop_type is a numbered list with indices c(1,2,3,4). Default: NULL

use_parallel
Boolean, whether to parallelise over the files using the mclapply from the parallel package.

Value

Named nested list of the same length as selections containg the loop data in the raw_cf format. Each named element corresponds to one loop type. For scalar-valued loop types, each element of the underlying numbered list corresponds to one momentum combination as specified via selections for this loop type in the same order. For the vector-valued loop types, the first level of the underlying numbered list has four elements corresponding to the four derivative directions in the order t,x,y,z. At the next level, the underlying numbered list corresponds to the momentum combinations for this loop type and derivative direction, just as for the scalar type.

disc_3pt

disconnected contribution to current insertion three-point function

Description

Computes the quark-line disconnected contribution to a three-point function of the form

$$C_3(t, \Delta t = t_{snk} - t_{src}) = C_2(t_{snk}, t_{src}) * L(t)$$

 $\forall t$ considering only the case $t_{snk} > t_{src}$.

Usage

```
disc_3pt(cf_2pt, loop, src_ts, dt, reim_loop = "both", reim_2pt = "both",
    vev_subtract = FALSE)
```

Arguments

| cf_2pt | 'raw_cf' container holding two-point part of three-point function in lattice-absolute coordinates (not relative to source!) |
|--------|--|
| loop | 'raw_cf' container holding loop contribution, suitably spin-projected and averaged over stochastic samples. |
| src_ts | Integer vector, the source time slices that were used for the computation of the two-point function in lattice-absolute coordinates. Must be of the same length as the number of measurements in cf_2pt. |
| dt | Integer, the source-sink separation that should be computed. |

dispersion_relation 65

| reim_loop | String, one of 'real', 'imag' or 'both'. Specifies whether just the real or imaginary part should be considered when constructing the correlation with the two-point function. |
|--------------|--|
| reim_2pt | String, same as reim_loop but for the two-point contribution to the three-point function. |
| vev_subtract | Boolean, whether the loop contains a vev which should be subtracted. |

Value

raw_cf container with the product of loop and 2pt function, shifted in time to be relative to source using the info from src_ts

dispersion_relation Continuum dispersion relation for CM to lattice frame

Description

Converts a center of mass (CM) frame energy to the lattice frame using the continuum dispersion relation.

Usage

```
dispersion_relation(energy, momentum_d, extent_space, plus = TRUE,
  lattice_disp = FALSE)
```

Arguments

energy double. CM energy in lattice units, aE.

momentum_d integer. Total momentum squared of the moving frame in lattice units, d^2 .

extent_space integer. Spatial extent of the lattice as a dimensionless quantity, L/a.

plus Boolean. Sign of a^2 artefacts.

lattice_disp Boolean. Use the lattice dispersion relation instead of the continuum one

Value

double. Energy in the lattice frame, aW.

double_bootstrap.cf

double_bootstrap.cf double bootstrap function for cf

Description

double bootstrap a set of correlation functions

Usage

```
double_bootstrap.cf(cf, dbboot.R = 99)
```

Arguments

cf bootstrapped correlation matrix of class cf obtained by a call to bootstrap.cf dbboot.R number of double bootstrap samples per original bootstrap sample

Value

returns an object of class cf unchanged from input but with double bootstrap samples added for the correlation function called doubleboot\$cf. Moreover, 'dbboot.R' is stored in the element doubleboot\$dbboot.R. Note that dbboot.R operations need to be performed per original bootstrap sample, so large dbboot.R might lead to very long execution time. The error of the correlation function is computed and stored as tsboot.sse in cf.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
tsboot, jab.cf, bootstrap.cf
```

```
data(samplecf)
samplecf <- bootstrap.cf(cf=samplecf, boot.R=10, boot.l=2, seed=1442556)
samplecf <- double_bootstrap.cf(cf=samplecf, dbboot.R=10)</pre>
```

effectivemass 67

| effectivemass | effectivemass |
|---------------|---------------|
|---------------|---------------|

Description

computes the effective mass with error analysis using UWerr

Usage

```
effectivemass(from, to, Time, Z, pl = TRUE, S, ...)
```

Arguments

```
from integer. Fit in fitrange (from, to)
to integer. see from.

Time integer. time extent of the lattice
Z data
pl boolean. plot
S numeric. see uwerr
... additional parameters passed to uwerr
```

Value

Returns a data.frame with named columns t, mass, dmass, ddmass, tauint and dtauint.

See Also

uwerr

```
effective mass values for a correlation function
```

Description

Computes effective mass values for a correlation function using different type of definitions for the effective mass. This function is mainly indented for internal usage by bootstrap.effectivemass.

```
effectivemass.cf(cf, Thalf, type = "solve", nrObs = 1,
  replace.inf = TRUE, interval = c(1e-06, 2), weight.factor = NULL,
  deltat = 1, tmax = Thalf - 1)
```

68 effectivemass.cf

Arguments

cf The correlation function either as a vector of length nr0bs*(Thalf+1) or as an

array of dimension Nxnr0bs*(Thalf+1), where N is the number of observa-

tions. N will be averaged over.

Thalf Half of the time extent of the lattice

type The function to be used to compute the effective mass values. Possibilities are

"acosh", "solve", "log", "temporal", "shifted", "weighted" and "power". While the first three assume normal cosh behaviour of the correlation function, "temporal" is designed to remove an additional constant stemming from temporal states in two particle correlation functions. The same for "subtracted" and "weighted", the latter for the case of two particle energies with the two particle having different energies. In the latter case only the leading pollution is removed by removeTemporal.cf and taken into account here. "power" assumes a power-

law decay instead of an exponential.

nr0bs The number of "observables" included in the correlator

replace.inf If set to TRUE, all Inf values will be replaced by NA. This is needed for instance

for bootstrap.effectivemass.

interval initial interval for the uniroot function when numerically solving for the effec-

tive mass.

weight.factor relative weight for type "weighted" only, see details

deltat time shift for shifted correlation functions

tmax t-value up to which the effective mass is to be computed

Details

A number of types is implemented to compute effective mass values from the correlation function:

```
"solve": the ratio
```

```
C(t+1)/C(t) = \cosh(-m*(t+1))/\cosh(-m*t)
```

is numerically solved for m(t).

"acosh": the effective mass is computed from

$$m(t) = a\cosh((C(t-1) + C(t+1))/(2C(t)))$$

Note that this definition is less tolerant against noise.

"log": the effective mass is defined via

$$m(t) = \log(C(t)/C(t+1))$$

which has artifacts of the periodicity at large t-values.

"temporal": the ratio

$$[C(t) - C(t+1)]/[C(t-1) - C(t)] = [\cosh(-m*(t)) - \cosh(-m*(t+1))]/[\cosh(-m*(t-1)) - \cosh(-m(t))]$$

is numerically solved for m(t).

"subtracted": like "temporal", but the differences C(t)-C(t+1) are assumed to be taken already at the correlator matrix level using removeTemporal.cf and hence the ratio

```
[C(t+1)]/[C(t)] = [\cosh(-m*(t)) - \cosh(-m*(t+1))]/[\cosh(-m*(t-1)) - \cosh(-m(t))] is numerically solved for m(t).
```

effmass 69

"weighted": like "subtracted", but now there is an additional weight factor w from removeTemporal.cf to be taken into account, such that the ratio

```
[C(t+1)]/[C(t)] = [\cosh(-m*(t)) - w*\cosh(-m*(t+1))]/[\cosh(-m*(t-1)) - w*\cosh(-m(t))]
```

is numerically solved for m(t) with w as input.

Value

Returns a vector of length Thalf with the effective mass values for t-values running from 0 to Thalf-1

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

arXiv:1203.6041

See Also

bootstrap.effectivemass

Examples

```
data(correlatormatrix)
cfnew <- extractSingleCor.cf(correlatormatrix, id=1)
cfnew <- bootstrap.cf(cfnew, boot.R=99, boot.l=1)
X <- effectivemass.cf(cfnew$cf, Thalf=25, tmax=24)</pre>
```

effmass

effmass

Description

computes the effective mass via the inverse cosh

Usage

```
effmass(data, timeextent, t)
```

Arguments

data numeric vector. data vector of length 4 timeextent integer. time extent of the lattice

t integer. physical time at which to evaluate the cosh

Value

Returns the effective mass as a single numeric value.

effmass2

effmass2

Description

computes the effective mass via the inverse cosh

Usage

```
effmass2(data, timeextent, t)
```

Arguments

data numeric vector. data vector of length 4 timeextent integer. time extent of the lattice

t integer. physical time at which to evaluate the cosh

Value

Returns the effective mass as a single numeric value.

escapeLatexSpecials

Escape special LaTeX characters for use in LaTeX labels

Description

Escape special LaTeX characters for use in LaTeX labels

Usage

```
escapeLatexSpecials(x)
```

Arguments

Х

String or vector of strings.

Value

String or vector of strings with all occurences of "#", "\$", "%", "&", "~", "_", "^", ">", "<" replaced by escaped counterparts which should render fine when used in a tikz plot, for example.

References

from https://stackoverflow.com/questions/36338629/escaping-special-latex-characters-in-r

extract.loop 71

| extract.loop Extract a single loop from an object of class cmiloop | extract.loop | Extract a single loop from an object of class cmiloop | |
|--|--------------|---|--|
|--|--------------|---|--|

Description

Extracts all loop values from an object of class cmiloop for all available times, samples and configurations.

Usage

```
extract.loop(cmiloop, obs = 9, ind.vec = c(2, 3, 4, 5, 6, 7, 8, 1), L)
```

Arguments

| cmiloop | input object of class cmiloop generated for instance with readcmiloopfiles. |
|---------|--|
| obs | the observable to extract |
| ind.vec | index vector to be used during extraction with ind.vec[1] the column with the observable number, ind.vec[2] the time values, ind.vec[3] the sample numbers, ind.vec[4] the real part of the local loop, ind.vec[5] the imaginary part of the local loop, ind.vec[6] and ind.vec[7] the same for fuzzed (or smeared) loops and ind.vec[8] for the configuration number. |

The spatial lattice extent needed for normalisation. If not given set to Time/2.

Value

L

a list with elements as follows:

cf: real part of the local loop

icf: imaginary part of the local loop scf: real part of the smeared loop

iscf: imaginary part of the smeared loop

Time=Time, nrSamples, nrObs=1, nrStypes=2, obs=obs and conf.index. The last is the list of configurations corresponding to the loops.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

readcmiloopfiles

72 extract.obs

| extract.obs | Extract One or More Gamma Combinations from am CMI Correlator |
|-------------|---|
| | |

Description

Extracts one or more gamma matrix combinations (observables) from a correlator stored in cmi format

Usage

```
extract.obs(cmicor, vec.obs = c(1), ind.vec = c(1, 2, 3, 4, 5), sym.vec,
    sign.vec, verbose = FALSE, symmetrise = TRUE)
```

Arguments

| cmicor | an correlator object in cmi format |
|------------|--|
| vec.obs | vector containing the numbers of observables to be extracted. |
| ind.vec | Index vector indexing the column numbers in cmicor to be used. The first must be the observable index, the second the smearing type index, the third the time, the fourth $C(+t)$ and the fifth $C(-t)$. |
| | Index vector indexing the column numbers in cmiloop to be used. The first must be the observable index, the second the smearing type index, the third the time, the fourth ReTL, the fifth ImTL, the sixth ReTF and the seventh ImTF. |
| sym.vec | a vector of bools of length equal to the number of observables indicating whether $C(t)$ is symmetric in t , i.e. whether $C(+t)$ and $C(-t)$ should be added or subtracted. If not given $C(+t)$ and $C(-t)$ will be assumed to be symmetric. |
| sign.vec | a sign vector of length equal to the number of observables indicating whether the corresponding correlation function should be multiplied by $+-1$. |
| verbose | Increases verbosity of the function. |
| symmetrise | if set to TRUE, the correlation function will be averaged for t and Time-t, with the sign depending on the value of sym. Note that currently the correlator with t-values larger than Time/2 will be discarded. |
| | |

Details

C(t) and C(-t) are averaged as indicated by sym.vec.

Value

cf

returns a list containing

for extract.obs: array containing the correlation function with dimension number of files times (nrObs*nrStypes*(Time/2+1)). C(t) and C(-t) are averaged according to sym.vec. for extract.loop: ReTL

extractSingleCor.cf 73

| icf | for extract.loop only: ImTL |
|------|---|
| scf | for extract.loop only: $\ensuremath{\text{ReTF}}$ |
| sicf | for extract.loop only: $\mbox{Im}\mbox{TF}$ |

Time The time extent of the correlation functions.

nrStypes The number of smearing combinations.

nr0bs The number of observables.

nrSamples for extrac.loop only: the number of samples found in the files.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readcmicor, readcmidatafiles,
```

Examples

extractSingleCor.cf

extract one single correlator object as cf object from a large cf object.

Description

cf objects are capable of storing several correlation functions in form of a correlation matrix. extractSingleCor.cf lets one extract one of them.

Usage

```
extractSingleCor.cf(cf, id = c(1))
```

Arguments

cf input object of class cf

id id of the correlators in cf to be extracted

Value

A cf object containing only the single correlator

Returns an object of class cf corresponding of the ids element in the input object cf

Author(s)

Carsten Urbach < curbach@gmx.de>

See Also

cf

extract_mass

generic function to extract a fitted mass

Description

One of the main analysis tasks in hadron is the estimation of energy levels or masses from correlation functions. The corresponding analysis functions return objects, typically lists, containing the masses or energy levels. extract_mass is a generic function to extrac such fitted mass values.

Usage

```
extract_mass(object)
```

Arguments

object

Object to extract the mass from.

Value

Numeric. The mass value.

```
extract_mass.effectivemassfit
```

specialisation of extract_mass to objects of type effectivemassfit

Description

specialisation of extract_mass to objects of type effectivemassfit

Usage

```
## S3 method for class 'effectivemassfit'
extract_mass(object)
```

Arguments

object

Object of type ${\tt effective massfit}$ to extract the mass from.

Value

Numeric. The mass value.

extract_mass.matrixfit 75

```
extract_mass.matrixfit
```

specialisation of extract_mass to objects of type matrixfit

Description

specialisation of extract_mass to objects of type matrixfit

Usage

```
## S3 method for class 'matrixfit'
extract_mass(object)
```

Arguments

object

Object of type matrixfit to extract the mass from.

Value

Numeric. The mass value.

fit.cosh

Fits a sum of several cosh-functions

Description

Performs a correlated fit of a sum of several cosh-functions $\sum_i a_i \cosh(m_i t)$ to data generated with bootstrap.effectivemass. Requires the same input and produces analogous output as fit.effectivemass. The fit itself is performed by bootstrap.nlsfit.

Usage

```
fit.cosh(effMass, cf, t1, t2, useCov = FALSE, m.init, par, n.cosh = 2,
  adjust.n.cosh = FALSE, every, ...)
```

Arguments

| effMass | An object of class effectivemass generated by a call to bootstrap.effectivemass. Either effMass or cf has to be provided, but not both! |
|---------|---|
| cf | An object of class cf_boot generated by a call to bootstrap.cf. Either cf or effMass has to be provided, but not both! |
| t1 | The fit range. If several correlators are fitted, this is automatically replicated accordingly. The fit range is adjusted such that NAs are removed from the fit. They must fulfill $t_1 < t_2$. For symmetric correlators, they must both run from 0 to T/2-1, otherwise from 0 to T-1. |

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| t2 | see t1 |
|---------------|---|
| useCov | Use the correlated chisquare. This works only for not too noisy data. |
| m.init | Initial guess of the effective mass, i.e. the smallest m_i. |
| par | Array of length $2*n$. cosh with initial guesses for the effective masses in the first n . cosh entries and initial guesses for the amplitudes in the last n . cosh entries. |
| n.cosh | Number of cosh-functions summed over. |
| adjust.n.cosh | Only relevant, if n.cosh=2. If set to TRUE, n.cosh can be adjusted to n.cosh=1 automatically in case the excited state cannot be resolved. |
| every | Fit only a part of the data points. Indices that are not multiples of every are skipped. If no value is provided, all points are taken into account. |
| | Additional parameters passed to the fit function. But the fit function is fixed and does not accept any arguments, so it will just crash. Therefore, don't use this! |

Value

An object with class coshfit is returned. It contains all the data of the input object effMass or the cf object as a member. The following member objects are added:

t0: the object returned by the optim on the original data. The format is as in par.

t: the bootstrap values of the results.

se: errors calculated via bootstrap on the results.

ii: the index array of data used in the fit.

invCovMatrix: the inverse covariance matrix.

dof: the degrees of freedom of the fit.

chisqr: Chi squared value of the fit.

Qval: p-value of the fit.

Author(s)

Johann Ostmeyer, <ostmeyer@hiskp.uni-bonn.de>

See Also

bootstrap.effectivemass, bootstrap.gevp, invertCovMatrix, bootstrap.nlsfit, fit.effectivemass

Examples

```
samplecf <- bootstrap.cf(cf=samplecf, boot.R=99, boot.l=2, seed=1442556)</pre>
effmass <- fit.cosh(bootstrap.effectivemass(cf=samplecf), t1=15, t2=23)</pre>
summary(effmass)
plot(effmass, ylim=c(0.14,0.15))
```

fit.effectivemass 77

| it.effectivemass Fits a constant to effective mass da |
|---|
|---|

Description

Performs a correlated fit of a constant to data generated with bootstrap.effectivemass.

Usage

```
fit.effectivemass(cf, t1, t2, useCov = FALSE, replace.na = TRUE,
boot.fit = TRUE, autoproceed = FALSE, every)
```

Arguments

| cf | $An \ object \ of \ class \ effective mass \ generated \ by \ a \ call \ to \ bootstrap. \ effective mass.$ |
|-------------|---|
| t1, t2 | The fit range. If several correlators are fitted, this is automatically replicated accordingly. The fit range is adjusted such that NAs are removed from the fit. They must fulfill $t_1 < t_2$. For symmetric correlators, they must both run from 0 to Time/2-1, otherwise from 0 to Time-1. |
| useCov | Use the correlated chisquare. This works only for not too noisy data. |
| replace.na | The functions inverted to determine the effective mass values might, due to fluctuations, return NA. If replace.na=TRUE, these are reaplaced in the bootstrap samples by randomly chosen values from the distribution that are not NA. Otherwise the fits in which the NA values occur will fail. |
| boot.fit | If set to FALSE, the effective mass fit is not bootstrapped, even though bootstrap samples are still used to estimate the variance-covariance matrix for the correlated fit. This is a useful time-saver if error information is not strictly necessary. Of course, this affects the return values related to the bootstrap, which are set to NA. |
| autoproceed | When the inversion of the variance-covariance matrix fails, the default behaviour is to abort the fit. Setting this to TRUE means that the fit is instead continued with a diagonal inverse of the variance-covariance matrix. |
| every | Fit only a part of the data points. Indices that are not multiples of every are skipped. If no value is provided, all points are taken into account. |

Details

A correlated chisquare minimisation is performed on the original data as well as on all bootstrap samples generated by bootstrap.effectivemass. The inverse covariance matrix is generated as described in hep-lat/9412087 in case of too little data to relibably estimate it.

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Value

An object with class effectivemassfit is returned. It contains all the data of the input object effMass with the following additional member objects:

```
{\tt opt.res:} the object returned by the optim on the original data.
```

massfit.tsboot: the bootstrap values of the mass and the chisquare function.

ii: the index array of data used in the fit.

invCovMatrix: the inverse covariance matrix.

dof: the degrees of freedom of the fit.

t1, t2: the fit range.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

C.Michael, A.McKerrell, Phys.Rev. D51 (1995) 3745-3750, hep-lat/9412087

See Also

bootstrap.effectivemass, bootstrap.gevp, gevp2cf, invertCovMatrix

Examples

```
data(samplecf)
samplecf <- bootstrap.cf(cf=samplecf, boot.R=99, boot.l=2, seed=1442556)
effmass <- fit.effectivemass(bootstrap.effectivemass(cf=samplecf), t1=15, t2=23)
summary(effmass)
plot(effmass, ylim=c(0.14,0.15))</pre>
```

fit.plateau2cf

fits a plateau to an object of class cf

Description

where applicable, a plateau is fitted to the averaged data in cf using a (correlated) chisquare fit.

Usage

```
fit.plateau2cf(cf, t1, t2, useCov = FALSE)
```

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Arguments

| cf | input object of class cf |
|----|------------------------------|
| t1 | starting t-value for the fit |
| t2 | final t-value for the fit. |

useCov perform a correlated chisquare fit or not.

Value

Returns a list with elements

plateau the fitted plateau value

dplateau its error

Author(s)

Carsten Urbach < curbach@gmx.de>

See Also

cf

Examples

```
data(correlatormatrix)
cfnew <- extractSingleCor.cf(correlatormatrix, id=1)
cfnew <- bootstrap.cf(cfnew, boot.R=99, boot.l=1)
X <- fit.plateau2cf(cfnew, t1=13, t2=20)</pre>
```

foldr1

Folds the non-empty list with the binary function

Description

A right fold without the need for a neutral element. Does not work with empty lists.

Usage

```
foldr1(f, xs)
```

Arguments

f function. A binary function that takes two elements of the type contained in

xs and returns another such element.

xs list or vector. Homogenious list or vector of elements.

There is a Reduce function in base R that does left and right folds. It always needs a starting element, which usually is the neutral element with respect to the binary operation. We do not want to specify such a neutral element for certain operations, like +.cf. Still a functional programming style should be supported

such that one can use maps and folds.

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Examples

```
# We generate some random numbers.
numbers <- rnorm(10)

# The sum is easiest computed with the `sum` function:
sum(numbers)

# If we wanted to implement `sum` ourselves, we can use a right fold to do
# so:
Reduce(`+`, numbers, 0.0)

# With this new function we do not need a neutral element any more, but give
# up the possibility to fold empty lists.
foldr1(`+`, numbers)</pre>
```

fs.a0

Finite Size Corrections to $q \cot \delta$ for $I=2 \pi \pi$ near threshold

Description

fs.qcotdelta computes the finite size corrections to $q \cot \delta$ while fs.mpia0 computes the corresponding finite size corrections to $M_\pi a_0$ directly using the Gasser Leutwyler result from M_π .

Usage

```
fs.a0(a0, mps, L)
```

Arguments

a0 scattering length at finite L

mps pion mass as a scalar variable (must not be a vector)

L spatial lattice extent as a scalar variable (must not be a vector)

Value

returns a numeric value representing the finite size correction or in case of fs. a0 the corrected value for a0.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

For the original formula see Eq. (31) from hep-lat/0601033

Examples

```
fs.a0(a0=1., mps=0.123, L=24)
```

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| _ | | | _ |
|-----|----|---|----|
| fs. | mn | 1 | аи |
| | | | |

Finite Size Corrections to $q \cot \delta$ for $I=2 \pi \pi$ near threshold

Description

fs.qcotdelta computes the finite size corrections to $q \cot \delta$ while fs.mpia0 computes the corresponding finite size corrections to $M_\pi a_0$ directly using the Gasser Leutwyler result from M_π .

Usage

```
fs.mpia0(mps, fps, L)
```

Arguments

mps pion mass as a scalar variable (must not be a vector)

fps pion decay constant as a scalar variable (must not be a vector)

L spatial lattice extent as a scalar variable (must not be a vector)

Value

returns a numeric value representing the finite size correction or in case of fs. a0 the corrected value for a0.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

For the original formula see Eq. (31) from hep-lat/0601033

Examples

```
fs.mpia0(mps=0.123, fps=0.2, L=24)
```

fs.qcotdelta

Finite Size Corrections to $q \cot \delta$ for I=2 $\pi\pi$ near threshold

Description

fs.qcotdelta computes the finite size corrections to $q\cot\delta$ while fs.mpia0 computes the corresponding finite size corrections to $M_\pi a_0$ directly using the Gasser Leutwyler result from M_π .

Usage

```
fs.qcotdelta(mps, L)
```

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Arguments

mps pion mass as a scalar variable (must not be a vector)

L spatial lattice extent as a scalar variable (must not be a vector)

Value

returns a numeric value representing the finite size correction or in case of fs. a0 the corrected value for a0.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

For the original formula see Eq. (31) from hep-lat/0601033

g1

Examples

```
fs.qcotdelta(mps=0.123, L=24)
```

g1

Description

Implementation of the Gasser-Leutwyler function g_1 for computing finite volume effects.

Usage

g1(x)

Arguments

x Numeric. x-value

getorderedconfignumbers

Creates an ordered vector of gauge config file numbers

Description

These functions generate an ordered list of config numbers by using a path and a basename and '*'.

Usage

```
getorderedconfignumbers(path = "./", basename = "onlinemeas",
  last.digits = 4, ending = "")
```

Arguments

path the path to be searched basename the basename of the files

last.digits the number of last characters in each filename to be used for ordering the list.

ending the file extension after the digits.

Details

All filenames are assumend to have equal length.

Value

returns the ordered list of gauge config numbers as a numeric vector.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readcmidatafiles, extract.obs
```

Examples

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getorderedfilelist

Creates an ordered filelist from a basename and a path

Description

These functions generate an ordered filelist and an order list of config numbers by using a path and a basename and '*'.

Usage

```
getorderedfilelist(path = "./", basename = "onlinemeas", last.digits = 4,
  ending = "")
```

Arguments

path the path to be searched basename the basename of the files

last.digits the number of last characters in each filename to be used for ordering the list.

ending the file extension after the digits.

Details

All filenames are assumend to have equal length.

Value

returns the ordered list of strings.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readcmidatafiles, extract.obs
```

Examples

get_plotdata_raw_cf 85

get_plotdata_raw_cf extract data from 'raw_cf' in format convenient to plot

Description

When dealing with with tensorial raw_cf objects pre-processing and reshaping is always required to prepare the data for plotting (or similar). This function conveniently prepares a named list of prepared data. The list elements are themselves lists which contain val and dval members with the central value and error of the element in question. These are in turn arrays of dimension c(cf\$nts, cf\$dim) and thus lack the first index compared to cf\$data.

Usage

```
get_plotdata_raw_cf(cf, reim, tauint, relerr)
```

Arguments

| cf | raw_cf object with meta-data and data. |
|--------|---|
| reim | String, one of 'real', 'imag' or 'both'. Specifies whether the real and/or imaginary parts should be extracted. |
| tauint | Boolean, specifies if the tensor of auto-correlation times and corresponding errors should be extracted. |
| relerr | Boolean, specifies if the return value should also include estimates of the relative |

error and its error.

Value

List of up to six named elements (depending on what was passed for reim, tauint, relerr) containing the central values and errors of the real and/or imaginary part of cf\$data as well as the corresponding arrays of auto-correlation times and relative errors. The list elements come in the order real, imag, relerr_real, relerr_imag, tauint_real, tauint_imag if reim is both and tauint and relerr are TRUE. The val and dval members of these list elements are arrays of dimension c(cf\$nts, cf\$dim) and thus lack the first index compared to cf\$data.

gevp solve GEVP for correlator matrix

Description

solve GEVP for a real, symmetric correlator matrix

Usage

```
gevp(cf, Time, t0 = 1, element.order = 1:cf$nrObs, for.tsboot = TRUE,
    sort.type = "vectors", sort.t0 = TRUE)
```

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Arguments

correlation matrix preferably obtained with a call to extrac. obs (or at leas with cf

the same structure) or an already averaged one.

cf is supposed to be an array of dim=c(N, n*(Time/2+1)), where N is the number of observations and n is the number of single correlators in the matrix. E.g.

for a 2x2 matrix n would be 4.

Time time extent of the lattice.

initial time value of the GEVP, must be in between 0 and Time/2-2. Default is t0

element.order specifies how to fit the n linearly ordered single correlators into the correlator

matrix. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order],

nrow=2).

for.tsboot for internal use of bootstrap.gevp. Alters the returned values, see details.

sort.type Sort the eigenvalues either in descending order, or by using the scalar product

of the eigenvectors with the eigenvectors at $t = t_0 + 1$. Possible values are

"values", "vectors" or "det".

if true (default), sort with respect to data at t0, otherwise with respect to t-1. sort.t0

Details

The generalised eigenvalue problem

 $C(t)v(t,t_0) = C(t_0)\lambda(t,t_0)v(t,t_0)$

is solved by performing a Cholesky decomposition of $C(t_0) = L^t L$ and transforming the GEVP into a standard eigenvalue problem for all values of t. The matrices C are symmetrised for all t. So we solve for λ

$$(L^t)^{-1}C(t)L^{-1}w = \lambda w$$

with

w = Lv or the wanted $v = L^{-1}w$.

The amplitudes can be computed from

 $A_i^{(n)}(t) = \sum_j C_{ij}(t) v_j^{(n)}(t,t_0) / (\sqrt{(v^{(n)},Cv^{(n)})(\exp(-mt)\pm \exp(-m(t-t)))}) \text{ and this is what the code returns up to the factor}$

 $1/\sqrt{\exp(-mt)} \pm \exp(-m(t-t))$ The states are sorted by their eigenvalues when "values" is chosen. If "vectors" is chosen, we take $\max(\sum_i \langle v(t_0, i), v(t, j) \rangle)$ with v the eigenvectors. For sort type "det" we compute max(...)

Value

Returns a list with the sorted eigenvalues, sorted eigenvectors and sorted (reduced) amplitudes for

In case for tsboot=TRUE the same is returned as one long vector with first all eigenvalues concatenated, then all eigenvectors and then all (reduced) amplitudes concatenated.

Author(s)

Carsten Urbach, <curbach@gmx.de>

gevp.hankel 87

References

Michael, Christopher and Teasdale, I., Nucl.Phys.B215 (1983) 433, DOI: 10.1016/0550-3213(83)90674-0
Blossier, B. et al., JHEP 0904 (2009) 094, DOI: 10.1088/1126-6708/2009/04/094, arXiv:0902.1265

See Also

boostrap.gevp, extract.obs

gevp.hankel

GEVP method based on Hankel matrices.

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input real numeric vector and a generalised eigenvalue problem is solved then.

Usage

```
gevp.hankel(cf, t0 = 1, deltat = 1, n, N, submatrix.size = 1,
  element.order = c(1, 2, 3, 4), Delta = 1, only.values = FALSE,
  custom.indices = NA, effTime = N)
```

Arguments

| cf | Numeric vector (this will generally be the time slices of a correlation function). |
|----------------|---|
| t0 | Integer. Initial time value of the GEVP, must be in between 0 and Time/2-2. Default is 1. |
| deltat | Integer. Time shift to be used to build the Hankel matrix |
| n | Integer. Size of the Hankel matrices to generate. This needs to include the factor of 'submatrix.size'. |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix |
| submatrix.size | Integer. Submatrix size to be used in build of Hankel matrices. Submatrix.size > 1 is experimental. |
| element.order | Integer vector. specifies how to fit the n linearly ordered single correlators into the correlator matrix for submatrix.size > 1. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Matrix elements can occur multiple times, such as c(1,2,2,3) for the symmetric case, for example. |
| Delta | integer. Delta is the time shift used in the Hankel matrix. |
| only.values | boolean. If 'TRUE', return only the eigenvalues, not the eigenvectors. |
| custom.indices | integer. Vector of indices to be using in cf instead of computing them from 'Delta' and 't0' |
| effTime | integer. Per default it is set to 'N'. It is only relevant for 'submatrix.size>1', and must contain the effective time extent of a single correlator, i.e. the spacing separating the different single correlator sequences in 'cf'. |

Value

A complex vector of length $n + n^2$ which contains the eigenvalues in the first n elements and the eigenvectors in the remaining n^2 elements. Unless 'only.values=TRUE' is set, when only the 'n' eigenvalues are returned in a complex vector of length n.

A vector of NAs of $n + n^2$ or n is returned in case the QR decomposition fails.

See Also

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

gevp.hankel_summed

GEVP method based on Hankel matrices.

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input real numeric vector and a generalised eigenvalue problem is solved then.

Usage

```
gevp.hankel_summed(cf, t0values = c(1), deltat = 1, n, N)
```

Arguments

| cf | Numeric vector (this will generally be the time slices of a correlation function). |
|----------|--|
| t0values | Integer vector. The t0 values to sum over. |
| deltat | Integer. The value of the time shift to use to build the Hankel matrices. |
| n | Integer. Size of the Hankel matrices to generate |
| | |

N Integer. Maximal time index in correlation function to be used in Hankel matrix

Value

A complex vector of length $n + n^2$ which contains the eigenvalues in the first n elements and the eigenvectors in the remaining n^2 elements.

A vector of NAs of n + n^2 is returend in case the QR decomposition fails.

See Also

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

gevp.truncated.hankel GEVP method based on truncated Hankel matrices.

Description

Alternative method to determine energy levels from correlation matrices. A so-called Hankel matrix is generated from an input real numeric vector, truncated via SVD and a generalised eigenvalue problem is solved then.

Usage

```
gevp.truncated.hankel(cf, t0 = 1, deltat = 1, n, N, max.truncation = n,
   submatrix.size = 1, element.order = c(1, 2, 3, 4), Delta = 1,
   get.coeffs = FALSE, effTime = N, error.weights = FALSE,
   symmetric = TRUE)
```

Arguments cf

| cf | Numeric vector (this will generally be the time slices of a correlation function). |
|----------------|---|
| t0 | Integer. Initial time value of the GEVP, must be in between 0 and Time/2-2. Default is 1. |
| deltat | Integer. Time shift to be used to build the Hankel matrix. |
| n | Integer. Size of the Hankel matrices to generate. This needs to include the factor of 'submatrix.size'. |
| N | Integer. Maximal time index in correlation function to be used in Hankel matrix. |
| max.truncation | Integer. Maximal truncation dimension to be used. Default is n*submatrix.size, the maximal possible value. |
| submatrix.size | Integer. Submatrix size to be used in build of Hankel matrices. Submatrix.size > 1 is experimental. |
| element.order | Integer vector. specifies how to fit the n linearly ordered single correlators into the correlator matrix for submatrix.size > 1. element.order=c(1,2,3,4) leads to a matrix matrix(cf[element.order], nrow=2). Matrix elements can occur multiple times, such as c(1,2,2,3) for the symmetric case, for example. |
| Delta | integer. Delta is the time shift used in the Hankel matrix. |
| get.coeffs | boolean. If 'TRUE', correlator coefficients are also calculated, not only the decay spectrum. |
| effTime | integer. Per default it is set to 'N'. It is only relevant for 'submatrix.size>1', and must contain the effective time extent of a single correlator, i.e. the spacing separating the different single correlator sequences in 'cf'. |
| error.weights | boolean or numeric vector. If 'FALSE', no error weighting is applied. If 'TRUE', the inverse standard error of the correlator is used as weights. If a numeric vector is given, it must be of the same length as cf\$cf0 and contains the weights to be used. |
| symmetric | boolean. If 'TRUE', the energy spectrum is guaranteed to be symmetric about 0. Default is cf\$symmetrised. |

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Value

List object containing the following entries:

cfii Integer vector. The time indices of the correlator used in the Hankel matrix.

spectrum Numeric matrix. The decay eigenvalues for truncation dimensions 1 to max.truncation.

singular.values

Numeric vector. The singular values of the full Hankel matrix, sorted by abso-

lute value.

coefficients (if get.coeffs=TRUE) Numeric array. The correlator coefficients for truncation

dimensions 1 to max.truncation.

See Also

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

gevp2amplitude

Extracts physical amplitudes from a GEVP

Description

Given a GEVP generated with bootstrap.gevp and masses determined from the principle correlator with given id, the physical amplitudes are extracted and bootstraped. The man amplitude is determined from a constant fit to the data in the specified time range.

Usage

```
gevp2amplitude(gevp, mass, id = 1, op.id = 1, type = "cosh", t1, t2,
  useCov = TRUE, fit = TRUE)
```

Arguments

| gevp | An object of class gevp as generated with a call to bootstrap.gevp. |
|-------|--|
| mass | Optimally, this is an object either of class effectivemassfit generated using fit.effectivemass or of class matrixfit generated with matrixfit to the principal correlator extracted using gevp2cf applied to gevp using the same value of id. |
| | It can also be given as a numerical vector with the bootstrap samples as entries. The mean will then be computed as the bootstrap mean over this vector. The number of samples must agree with the number of bootstrap samples in gevp. |
| id | The index of the principal correlator to extract, i.e. the physical state to extract. |
| op.id | The index of the operator for which to extract the amplitude. |
| type | The symmetry of the pricipal correlator in time, can be either "cosh" or "sinh". |
| | |

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| t1, t2 | The time range in which to fit the amplitude starting with 0. If not given it will be tried to infer these from the mass object. |
|--------|--|
| useCov | Use the covariance matrix for fitting the constant to the amplitude data. |
| fit | perform a fit to the data. |

Value

Returns an object of S3 class gevp.amplitude, generated as a list with named elements amplitude the numeric vector of amplitudes, amplitude.tsboot the corresponding bootstrap samples, damplitude the estimates for the standard errors, fit the object returned by the fit routine, meanAmplitude and meanAmplitude.tsboot mean amplitude and its bootstrap samples, chisqr the residual sum of squares, dof the numberi of degrees of freedom, t1 and t2 the fit range, and then all the input objects.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
matrixfit, fit.effectivemass, gevp, gevp2cf, computefps
```

Examples

```
data(correlatormatrix)
## bootstrap the correlator matrix
correlatormatrix <- bootstrap.cf(correlatormatrix, boot.R=99, boot.l=1, seed=132435)</pre>
## solve the GEVP
t0 <- 4
correlator matrix. gevp <-\ bootstrap. gevp (cf=correlator matrix, \ t0=t0, \ element. order=c(1,2,3,4))
## extract the ground state and plot
pion.pc1 <- gevp2cf(gevp=correlatormatrix.gevp, id=1)</pre>
pion.pc1.effectivemass <- bootstrap.effectivemass(cf=pion.pc1, type="solve")</pre>
pion.pc1.effectivemass <- fit.effectivemass(pion.pc1.effectivemass, t1=8, t2=23,</pre>
                                               useCov=FALSE)
## now determine the amplitude
pion.pc1.amplitude <- gevp2amplitude(correlatormatrix.gevp, pion.pc1.effectivemass,</pre>
                                       useCov=FALSE, t1=8, t2=14)
plot(pion.pc1.amplitude)
summary(pion.pc1.amplitude)
```

gevp2cf

Extracts a principle correlator from a GEVEP

Description

Extracts a principle correlator from a GEVP and converts it into an object of class cf

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Usage

```
gevp2cf(gevp, id = 1)
```

Arguments

gevp An object returned by bootstrap. gevp.

id The index of the principal correlator to extract.

Value

An object of class cf, which contains bootstrap samples already. So a call to bootstrap.cf is neither needed nor possible. It can be treated further by bootstrap.effectivemass or matrixfit to extract a mass value.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
gevp, matrixfit, bootstrap.effectivemass
```

Examples

```
data(correlatormatrix)
## bootstrap the correlator matrix
correlatormatrix <- bootstrap.cf(correlatormatrix, boot.R=99, boot.l=1, seed=132435)
## solve the GEVP
t0 <- 4
correlatormatrix.gevp <- bootstrap.gevp(cf=correlatormatrix, t0=t0, element.order=c(1,2,3,4))
## extract the ground state and plot
pc1 <- gevp2cf(gevp=correlatormatrix.gevp, id=1)
plot(pc1, log="y")</pre>
```

gm

List of arrays of gamma structures

Description

List of arrays of 4x4 complex gamma matrices in the tmLQCD chiral gamma basis, where $\gamma^5 = \gamma^0 \gamma^1 \gamma^2 \gamma^3 = \text{diag}(c(1,1,-1,-1))$ and the UKQCD gamma basis, where $\gamma^5 = \gamma^0 \gamma^1 \gamma^2 \gamma^3$.

The index mappings are as follows

```
• gm[['chiral_tmlqcd']][1,,] \gamma^0
```

- gm[['chiral_tmlqcd']][2,,] γ^1
- gm[['chiral_tmlqcd']][3,,] γ^2

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```
• gm[['chiral_tmlqcd']][4,,] \gamma^3
```

- gm[['chiral_tmlqcd']][5,,] γ^5
- gm[['chiral_tmlqcd']][6,,] positive parity projector $\frac{1}{2}(1+\gamma^0)$
- gm[['chiral_tmlqcd']][7,,] negative parity projector $\frac{1}{2}(1-\gamma^0)$
- gm[['ukqcd']][1,,] γ^1
- gm[['ukqcd']][2,,] γ^2
- gm[['ukqcd']][3,,] γ^3
- gm[['ukqcd']][4,,] γ^4
- gm[['ukqcd']][5,,] γ^5
- gm[['ukqcd']][6,,] positive parity projector $\frac{1}{2}(1+\gamma^4)$
- gm[['ukqcd']][7,,] negative parity projector $\frac{1}{2}(1-\gamma^4)$

The function gm_mu can be used to access its elements using a more "natural" indexing.

gm_mu

Accessor function for gm

Description

Retrieve the entries of the gm list of three-index arrays containing various gamma structures in a natural indexing.

Usage

```
gm_mu(mu, basis = "chiral_tmlqcd")
```

Arguments

mu

Number or string denoting

- Lorentz index (0,1,2,3,4) for γ^{μ}
- 5 for γ^5
- "Pp" or "Pm" for the positive and negative parity projectors respectively

basis

String, gamma basis to use. Possible values

'ukqcd': UKQCD gamma basis with $\gamma^i, i \in [1, 2, 3, 4]$ and $\gamma^5 = \gamma^1 \gamma^2 \gamma^3 \gamma^4$, such that 1 = x, 4 = t.

'chiral_tmlqcd': Chiral gamma basis used by tmLQCD with $\gamma^\mu, \mu \in [0,1,2,3]$ and $\gamma^5 = \gamma^0 \gamma^1 \gamma^2 \gamma^3$, such that $0=t,\,3=z$.

Value

Returns the requested γ matrix as a 4x4 complex valued array, see gm.

94 h5_names_exist

h5_get_dataset get dataset from HDF5 file

Description

get dataset from HDF5 file

Usage

```
h5_get_dataset(h5f, key, check_exists = TRUE)
```

Arguments

h5f HDF5 file opened with rhdf5::H5Fopen

key String, full path to dataset.

check_exists Boolean, check if key actually exists (keep in mind overhead).

Value

Returns the requested dataset, if successfully read from file.

h5_names_exist check if group names exist in HDF5 file

Description

The group names in an HDF5 file are stored as full paths as well as a flat vector. It is thus possible to check if a particular set of group names exist in the file by parsing the name member of the output of rhdf5::h5ls. This function does just that.

Usage

```
h5_names_exist(h5f, nms_to_find)
```

Arguments

h5f HDF5 file handle openend with rhdf5::H5Fopen

nms_to_find Vector of strings, group names (not full paths) which are to be located in the file.

Value

Vector of booleans of the same length as nms_to_find indicating whether the name at the same index position was located in the file.

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hadron

The Hadron Package

Description

An R implementation of fitting routines used in lattice QCD. It provides useful functions for extraction hadronic quantities and such like.

Details

Toolkit to perform statistical analyses of correlation functions generated from Lattice Monte Carlo simulations. In particular, a class cf for correlation functions and methods to analyse those are defined. This includes (blocked) bootstrap and jackknife, but also an automatic determination of integrated autocorrelation times. hadron also provides a very general function bootstrap.nlsfit to bootstrap a non-linear least squares fit. More specific functions are provided to extract hadronic quantities from Lattice Quantum Chromodynamics simulations, a particular Monte Carlo simulation, (see e.g. European Twisted Mass Collaboration, P. Boucaud et al. (2008) doi:10.1016/j.cpc.2008.06.013). Here, to determine energy eigenvalues of hadronic states, specific fitting routines and in particular the generalised eigenvalue method (see e.g. B. Blossier et al. (2009) doi:10.1088/11266708/2009/04/094 and M. Fischer et al. (2020) https://inspirehep.net/literature/1792113) are implemented. In addition, input/output and plotting routines are available.

Author(s)

Carsten Urbach, <urbach@hiskp.uni-bonn.de>

hankel2cf

hankel2cf

Description

hankel2cf

Usage

```
hankel2cf(hankel, id = c(1), range = c(0, 1), eps = 1e-16,
    sort.type = "values", sort.t0 = TRUE)
```

Arguments

hankel object as returned from bootstrap.hankel

id Integer. Index of eigenvalue to consider, $1 \le id \le n$.

range Numeric vector. Value-range for the real part of the eigenvalues (not the ener-

gies). If outside this range, the eigenvalue will be discarded

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| eps | Numeric. Cut-off: if the imaginary part of the generalised eigenvalues is larger than eps, the eigenvalue is discarded. |
|-----------|--|
| sort.type | the sort algorithm to be used to sort the eigenvalues. This can be either simply "values", or the eigenvector information is used in addition with "vectors" |
| sort.t0 | Boolean. Whether to use the eigenvector at t0 or the one at deltat-1 for sorting |

Value

Returns an object of S3 class cf.

See Also

input is generated via bootstrap.hankel alternatively use hankel2effectivemass. For the cf class see cf

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

hankel2effectivemass hankel2effectivemass

Description

hankel2effectivemass

Usage

```
hankel2effectivemass(hankel, id = c(1), type = "log", range = c(0, 1), eps = 1e-16, sort.type = "values", sort.t0 = TRUE, probs = c(0.16, 0.84), errortype = "normal", bias_correction = FALSE)
```

Arguments

| hankel | object as returned from bootstrap.hankel |
|-----------|--|
| id | Integer. Index of eigenvalue to consider, $1 \le id \le n$. |
| type | Character vector. Type of effective mass to use. Must be in c("log", "acosh") |
| range | Numeric vector. Value-range for the real part of the eigenvalues (not the energies). If outside this range, the eigenvalue will be discarded |
| eps | Numeric. Cut-off: if the imaginary part of the generalised eigenvalues is larger than eps, the eigenvalue is discarded. |
| sort.type | the sort algorithm to be used to sort the eigenvalues. This can be either simply "values", or the eigenvector information is used in addition with "vectors" |
| sort.t0 | Boolean. Whether to use the eigenvector at t0 or the one at deltat-1 for sorting |
| probs | numeric. Bector of probabilities. |

errortype

string. Determines the treatment of the bootstrap histograms to determine the statistical error on eigenvalues. Can be: 1. 'outlier-removal' for which outliers are removed according to the 0.25 and 0.75 quantiles and the inter-quantile-range, i.e. only values are kept which are in the interval $[Q_25-1.5IQR,Q_75+1.5IQR]$ and the error is computed from the standard deviation of the bootstrap distribution. 2. 'quantiles' for which the error is estimated from the difference between the 0.16 and 0.84 quantile of the original bootstrap distribution

bias_correction

boolean. If set to 'TRUE', the median of the bootstrap distribution is used as estimator for the energy values.

Value

Returns an object of S3 class effectivemass.

See Also

input is generated via bootstrap.hankel alternatively use hankel2cf. See also bootstrap.effectivemass

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), pgevm2bootstrapfit(), pgevm2effectivemass(), plot_hankel_spectrum()

hankeldensity2effectivemass

hankeldensity2effectivemass

Description

computes the density of all bootstrap replicates of effective masses

Usage

hankeldensity2effectivemass(hankel, range = c(0, 1), method = "median")

Arguments

hankel object as returned from bootstrap.hankel

range Numeric vector. Value-range for the real part of the eigenvalues. If outside this

range, the eigenvalue will be discarded

method Character vector. Method to be used to determine the central value of the effec-

tive mass. Must be "median" (default) or "density"

Value

Returns an object of S3 class effectivemass. #'

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See Also

bootstrap.effectivemass, hankel2effectivemass

has_icf

Checks whether the cf object contains an imaginary part

Description

Checks whether the cf object contains an imaginary part

Usage

```
has_icf(.cf)
```

Arguments

.cf

cf object

Value

Returns TRUE if the .cf object has an element icf, which is the imaginary component of the correlation function.

idx_matrix.raw_cf

Construct the tensor index set for the entire raw correlator

Description

Construct the tensor index set for the entire raw correlator

Usage

```
idx_matrix.raw_cf(cf, component)
```

Arguments

cf 'raw_cf' container with data and meta-data

component Integer vector. Optional argument to obtain a subset of the index matrix to access

a particular element of the interior dimensions. Must of the same length as

cf\$dim.

Value

An object of type matrix is returned containing the tensor index set.

int_idx_matrix.raw_cf 99

int_idx_matrix.raw_cf Construct tensor index set for the internal degrees of freedom

Description

Construct tensor index set for the internal degrees of freedom

Usage

```
int_idx_matrix.raw_cf(cf)
```

Arguments

cf

raw_cf container

Value

Returns a matrix containing the above mentioned index set.

Description

When a correlation function is modified, any resampling should be invalidated. We could instead also choose to properly work with the samples, but most computations are done with the original data anyway.

Usage

```
invalidate.samples.cf(cf)
```

Arguments

cf

cf object.

Value

Returns an object of class cf with all resampling removed.

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invcosh

numerically invert the cosh function for the mass

Description

numerically invert the cosh function for the mass

Usage

```
invcosh(ratio, timeextent, t, eps = 1e-09, maxiterations = 1000)
```

Arguments

ratio Numeric. The value of the ratio.
timeextent Integer. Time extent of the lattice.

t Integer. The t-value where the ratio was taken.

eps Numeric. Precision of the numerical solution

maxiterations Integer. Maximal number of iterations to be used in the iterative solver.

Value

A single numeric value is returned corresponding to the mass.

Examples

```
invcosh(1.2, timeextent=24, t=12)
```

invertCovMatrix

Inverts the covariance matrix for noisy data

Description

The covariance matrix of noisy data is inverted. Special care is taken in treating spurious small modes of the matrix, which are likely to arise from too much noise in the data.

Usage

```
invertCovMatrix(cf, boot.l = 1, boot.samples = FALSE, cov_fn = cov)
```

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Arguments

| cf | The data for which the covariance matrix is to be computed. It is expected to be an array or matrix with dimension RxN, where R is the number of observations and N the number of observables. |
|--------------|--|
| | cf can be either real data or bootstrap data. In the latter case boot.samples=TRUE must be set for proper normalisation of the inverse matrix. |
| boot.1 | If set to a value larger than 1 the data will be blocked with blocklength boot.1 before the covariance matrix is computed. |
| boot.samples | If set to TRUE the data is treated a pseudo data from a bootstrap procedure. |
| cov_fn | Function that computes the covariance matrix from the given samples. |

Details

The inverse covariance matrix is estimated. If the number of observations is too small the procedure described in the reference is used to remove spuriously small eigenvalues of the covariance matrix.

We always keep the \sqrt{R} largest eigenvalues exactly and replace the remaining smallest ones by their mean.

Value

Returns the inverse covariance matrix as an object of class matrix.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

C.Michael, A.McKerrell, Phys.Rev. D51 (1995) 3745-3750, hep-lat/9412087

See Also

```
cov, matrix
```

Examples

```
X <- array(rnorm(4000), dim=c(1000, 4))
invertCovMatrix(cf=X, boot.samples=TRUE)
M <- invertCovMatrix(cf=X, boot.samples=TRUE)
M</pre>
```

is.raw_cf

is.cf

Checks whether an object is a cf

Description

Checks whether an object is a cf

Usage

```
is.cf(x)
```

Arguments

Χ

Object, possibly of class cf.

Value

Returns TRUE if the input object is of class cf, FALSE otherwise.

is.raw_cf

check if an object is of class raw_cf

Description

check if an object is of class raw_cf

Usage

```
is.raw_cf(x)
```

Arguments

Х

object to be checked

Value

Returns TRUE if x is an object of class raw_cf, FALSE otherwise.

is_empty.cf

is_empty.cf

Checks whether the cf object contains no data

Description

Checks whether the cf object contains no data

Usage

```
is_empty.cf(.cf)
```

Arguments

.cf

cf object.

Value

returns FALSE if . cf contains no data, TRUE otherwise

Examples

```
# The empty cf object must be empty:
is_empty.cf(cf())
# The sample cf must not be empty:
is_empty.cf(samplecf)
```

is_empty.raw_cf

check if an obect is of class raw_cf and empty otherwise

Description

check if an obect is of class raw_cf and empty otherwise

Usage

```
is_empty.raw_cf(x)
```

Arguments

Х

object to be checked

Value

Returns TRUE if x is an empty object of class raw_cf, FALSE otherwise.

jackknife-after-bootstrap

jackknife-after-bootstrap analysis

Description

jackknife-after-bootstrap (JAB) analysis for errors of errors of correlation functions of class cf.

We apply the jackknife-after-bootstrap method as proposed by Efron (1992) for iid data and extended by Lahiri (2002) for dependent data. Blocks of bootstrap samples are deleted for a jackknife analysis. The jackknife replicates are computed from the bootstrap samples in which the corresponding block of blocks is missing.

We use here the moving blocked bootstrap (MBB) which uses overlapping blocks. The estimate of standard error of the bootstrap error is computed using formula (2.3) from Lahiri, 2002:

$$var_{jab} = (m(N-m)^{-1})M^{-1} \sum_{i=1}^{M} (\tilde{t}_n^{(i)} - \hat{t}_n)^2$$

with

$$\tilde{t}_n^{(i)} = m^{-1}(N\hat{t}_n - (N-m)\hat{t}_n^{(i)}).$$

Here, \hat{t}_n is the MBB estimate (in our case of standard deviation) and $\hat{t}_n^{(i)}$ is the i-th jackknife replication of it.

Arguments

cf An object of class cf generated by bootstrap.cf with sim="fixed".

m denotes the number of (overlapping) blocks to delete for the JAB analysis.

Value

Returns an object of class cf with an element jack.boot.se, which is the JAB estimate of standard error of the standard error.

Author(s)

Carsten Urbach < curbach@gmx.de>

References

S.N. Lahiri, "On the jackknife-after-bootstrap method for dependent data and its consistency properties", Econometric Theory, 2002, Vol. 18, 79-98

See Also

bootstrap.cf, cf, jackknife.cf

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jackknife.cf

jackknife a set of correlation functions

Description

jackknife a set of correlation functions

Usage

```
jackknife.cf(cf, boot.l = 1)
```

Arguments

cf correlation matrix of class cf e.g. obtained with a call to extrac.obs.

boot.1 block size for autocorrelation analysis

Value

returns an object of class cf with blocked jackknife samples added for the correlation function called cf.jackknife. Currently, only the moving block jackknife approach is implemented. Moreover, the original average of cf is returned as cf0 and the bootstrap errors as jackknife.se. We also copy the input parameters over and set jackknife.samples to TRUE.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

H.R. Künsch, "The jackknife and the bootstrap for general stationary observations", The Annals of Statistics, 1989, Vol. 17, No. 3, 1217-1241

S.N. Lahiri, "On the jackknife-after-bootstrap method for dependent data and its consistency properties", Econometric Theory, 2002, Vol. 18, 79-98

See Also

```
boot::tsboot,bootstrap.cf
```

Examples

```
data(samplecf)
samplecf <- jackknife.cf(samplecf, boot.l=1)
plot(samplecf, log="y")</pre>
```

jackknife_error

jackknife_cov

jackknife_cov

Description

Computes covariance matrix for jackknife samples.

Usage

```
jackknife_cov(x, y = NULL, na.rm = FALSE, ...)
```

Arguments

x a numeric vector, matrix or data frame.

y 'NULL' (default) or a vector, matrix or data frame with compatible dimensions

to 'x'. The default is equivalent to 'y = x' (but more efficient).

na.rm logical. The rows containing any NA will be deleted if this option is set.

... parameters to be forwarded to cov.

Value

returns a matrix corresponding to the jackknife estimate of the covariance matrix

jackknife_error

Estimates error from jackknife samples

Description

Computes the jackknife error which is just

$$\sum_{i=0}^{N} (x_i - \bar{x})^2.$$

Internally we use

$$\frac{(N-1)^2}{N}\operatorname{sd}(X)$$

in order to benefit from the optimized standard deviation function.

The width of the bootstrap distribution does not change with the number of elements. The jackknife distribution crucially depends on the number of measurements that one started with. Therefore we cannot just drop the NA values and are done with it. Instead we need to rescale with the $\sqrt{N/m}$ where N is the number of original measurements and m is the number of non-NA values. With NA values removed we would otherwise underestimate the uncertainty.

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Usage

```
jackknife_error(samples, boot.l = 1, na.rm = FALSE)
```

Arguments

samples Numeric vector.

boot.1 Block length for bootstrapping.

na.rm Logical. Determines whether NA values shall be removed, see Description for

details.

Details

Currently this uses the mean over the jackknife samples in order to compute the error. It would be better in the case of a bias to use the mean over the original data instead. This would require a second parameter and therefore is incompatible with the previously used sd everywhere for the bootstrap samples. As the sd for the bootstrap samples also does not include the original data, this likely is similar in terms of bias.

Value

returns a single numeric representing the jackknife estimate of error

|--|

Description

blub ...

Usage

```
lanczos.solve(cf, N, pivot = FALSE, pivot_elements = NULL)
```

Arguments

| cf | Numeric vector (this will generally be a correlation function or a bootstrap sample thereof). |
|----------------|---|
| N | Integer. Maximal time index in correlation function to be used in Lanczos analysis |
| pivot | boolean. whether or not to use a pivot element. |
| pivot_elements | numeric. the value(s) of the pivot elements. |

Value

tbw

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See Also

Other lanczos: bootstrap.lanczos()

loopdata

Sample loop data

Description

Sample data for fermion loops for a 24 cube times 48 lattice QCD simulation. It is stored in form of a list.

Format

```
list of 10 elements: "nrObs" "Time" "nrStypes" "symmetrised" "cf" "icf" "scf" "iscf" "nrSamples" "obs"
```

Examples

```
data("loopdata")
```

loop_2pt

compute two-point correlation function between quark loops

Description

compute two-point correlation function between quark loops

Usage

```
loop_2pt(loop_snk, loop_src, random_vectors_outer_product = FALSE,
   nstoch_to_avg = "all")
```

Arguments

loop_snk 'raw_cf' container with spin-projected quark loop at sink (see loop_spin_project) loop_src 'raw_cf' container with spin-projected quark loop at source (see loop_spin_project) random_vectors_outer_product

Boolean. For testing purposes, the average over all random sample combinations can be carried out explicitly as $\sum_{i\neq j} Tr[\Gamma_s nkM_i]Tr[\Gamma_s rcM_j]$ instead of the (much faster) equivalent $(\sum_i Tr[\Gamma_s nkM_i])*(\sum_j Tr[\Gamma_s rcM_j])-\sum_i (Tr[\Gamma_s nkM_i]Tr[\Gamma_s rcM_j])$.

String or integer, how many of the available stochastic samples should be aver-

nstoch_to_avg String or integer, how many of the available stochastic

aged over. See loop_stochav for details.

Value

'raw_cf' container with two-point function of these two quark loops. In the calculation, both averaging over all source locations and the average over all stochastic sample combinations are performed.

loop_spin_project 109

| loop_spin_project | spin projection of quark loop data |
|---------------------|------------------------------------|
| TOOD SDILL DLO LECT | SDIN DIVIECTION OF QUARK 100D adia |
| | |

Description

Implements the operation

$$L = a * (\Gamma_{ik} M_{ki})$$

to give the trace of a quark loop M multiplied by a gamma structure Γ and scaled by a complex factor a.

Usage

```
loop_spin_project(loop, gamma, reim = "both", stochav = FALSE,
    scale_factor = as.complex(1), herm_conj = FALSE)
```

Arguments

| loop | 'raw_cf' container with loop data |
|---------|--|
| gamma | 4x4 complex matrix |
| reim | String, one of 'real', 'imag' or 'both'. After the spin projection and trace, the result can be restricted to just the real or imaginary part, if desired. Useful for the cases in which it is clear that only one or the other contains any signal. |
| stochav | Boolean, specifies whether the average over stochastic samples should be performed. This makes the projection much faster but of course prevents the projected loop data to be used for the construction of diagrams with multiple quark loops. |

scale_factor Complex scaling factor to be applied.

herm_conj Boolean, optionally the loop matrix M can be hermitian conjugated before the

spin projection is performed.

Value

Returns an object of class raw_cf.

|--|

Description

Perform mean over the third dimension of the loop data.

Usage

```
loop_stochav(loop, nstoch_to_avg = "all")
```

loop_vev_subtract

Arguments

loop 'raw_cf' container with loop data

nstoch_to_avg String or integer, number of stochastic samples to average over. Only possi-

ble string is 'all'. If an integer is supplied, it must be at least '1' and at most

consistent with the number of stochastic samples in loop.

Value

Returns the input loop object with named elemens data and dim added.

loop_vev_subtract

subtract vev from loop data

Description

Convenience function to subtract any possible vacuum-expectation value from a loop matrix. The expectation value of each component of the internal dimensions is subtracted individually. Averaging over stochstic samples can be restricted to a subset, see nstoch_to_avg input parameter.

Usage

```
loop_vev_subtract(loop, nstoch_to_avg = "all")
```

Arguments

loop 'raw_cf' container with loop data

nstoch_to_avg String or integer, number of stochastic samples to average over. Only possi-

ble string is 'all'. If an integer is provided it must be at least '1' and at most

consistent with the number of stochastic samples in loop.

Value

Returns the input loop object with added data.

make_parind 111

| make_parind | make_parind | Create a parameter index matrix for matrixfit | |
|-------------|-------------|---|--|
|-------------|-------------|---|--|

Description

Create a parameter index matrix for matrixfit

Usage

```
make_parind(parlist, length_time, summands = 1)
```

Arguments

parlist integer array. Parameter list generated with make_parlist.

length_time integer. Number of time slices per correlator.

summands integer. Number of summands in the fit model that shall be fitted. The signal

counts as one summand, each explicit pollution term with independent ampli-

tudes counts as its own summand.

Value

Returns an array with the parameter indices.

Description

Create a parameter list for matrixfit

Usage

```
make_parlist(corr_matrix_size)
```

Arguments

```
corr_matrix_size
```

integer. Number of correlators in the matrix. This must be a the square of an integer.

Value

Returns a square, integer-valued matrix.

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matrixfit

Routine For A Factorising Matrix Fit

Description

Performs a factorising fit on a correlation matrix

Usage

```
matrixfit(cf, t1, t2, parlist, sym.vec, neg.vec, useCov = FALSE,
  model = "single", boot.fit = TRUE, fit.method = "optim",
  autoproceed = FALSE, every)
```

Arguments

| cf | correlation matrix obtained with a call to extrac.obs. |
|----------|---|
| t1 | lower bound for the fitrange in time (t1,t2). Counting starts with 0. |
| t2 | upper bound for the fitrange in time (t1,t2). Counting starts with 0. |
| parlist | a two dimensional array of dimension 2 times number of correlators in cf. Every column assigns a pair of fit parameters to the corresponding correlator in cf. In case this is missing there are defaults provided for certain matrix sizes. |
| sym.vec | a vector of length number of correlators in cf indicating whether the correlation function is a cosh, a sinh or an exponential. Possible values are "cosh", "sinh" and "exp". In case this is missing there are defaults provided for certain matrix sizes. |
| neg.vec | a vector of length number of correlators in cf indicating whether the correlation function is to be multiplied globally with a minus sign. In case this is missing there are defaults provided for certain matrix sizes. |
| useCov | use correlated or uncorrelated chisquare. Default is useCov=FALSE. |
| model | Sets the fit model to be used in the fit. The default model is $0.5p_ip_j(\exp(-Et)\pm c*\exp(-E(Time-t)))$ with sign depending on "cosh" or "sinh". c equals one except for the "exp" functional dependence. When model is set to "shifted", the fit uses the function $p_ip_j(\exp(-E(t+1/2))\mp c*\exp(-E(Time-(t+1/2))))$ which is useful when the original correlation function or matrix is shifted, see e.g. bootstrap.gevp. In case only a single principal correlator from a GEVP is to be fitted the additional model "pc" is available. It implements $\exp(-E(t-t_0))(A+(1-A)\exp(-DeltaE(t-t_0)))$ |
| | with t_0 the reference timesclice of the GEVP. See bootstrap.gevp for details. |
| boot.fit | If set to FALSE, the fit is not bootstrapped, even if the bootstrapping parameters |

boot.fit

If set to FALSE, the fit is not bootstrapped, even if the bootstrapping parameters have been set and the correlation function has been bootstrapped. This is a useful time-saver if error information is not strictly necessary. Of course, this affects the return values related to the bootstrap, which are set to NA.

matrixfit 113

fit.method Can be either "optim" or "lm". The latter works only if the library "minpack.lm"

can be loaded. Default and fallback is "optim".

autoproceed When the inversion of the variance-covariance matrix fails, the default behaviour

is to abort the fit. Setting this to TRUE means that the fit is instead continued with

a diagonal inverse of the variance-covariance matrix.

every Fit only a part of the data points. Indices that are not multiples of every are

skipped. If no value is provided, all points are taken into account.

Details

The routine expects in cf\$cf a set of correlation functions. The mapping of this linear construct to a matrix or a part of a matrix is achieved via parlist. The symmetry properties of the individual correlation functions must be encoded in sym.vec.

matrixfit will fit to every correlator in cf\$cf a function $p_i p_j f(t)$. The indices i, j are determined from parlist and f is either cosh or sinh, depending on sym.vec.

The inverse covariance matrix is computed using a singular value decomposition. If the sample size N is too small, only sqrt(N) eigenvalues of the matrix are kept exactly, while all others are replaced by the mean of the rest. This helps to reduce instabilities induced by too small eigenvalues of the covariance matrix.

Value

returns an object of class matrixfit with entries:

CF object of class cf which contains the mean correlation functions

M inverse variance-covariance matrix for weighted Chi squared minimization

L squre root of M.

parind indices in the parameter vector used for the different matrix combinations

sign.vec vector of signs

ii vector of vector indices giving the columns of the correlation function arrays

(CF above, say), which are contained in the fit range

opt.res return value of the minimization (see ?optim) on the original data.

Result of the chisqr fit on the original data. t0 is a vector of length npar+1,

where npar the number of fit parameters. The last value is the chisqr value.

t Bootstrap samples of the R Chi squared minimizations of length(par)+1. t has

dimension Rx(npar+1), where R is the number of bootstrap samples and npar the number of fit parameters. The last column corresponds to the chisquare

values.

se Bootstrap estimate of standard error for all parameters. se is a vector of length

npar, where npar the number of fit parameters.

useCov whether covariances in the data were taken into account

invCovMatrix inverse of covariance matrix or inverse variance weighted if useCov=FALSE

Qval real number between 0 and 1 giving the "quality" of the fit

chisqr total Chi squared of the fit

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dof fit degrees of freedom mSize integer size of the matrix which was fitted cf object of type cf which contains, amongst other objects, cf\$cf which is a concatenated array of raw correlation functions where each row is one of N observations and there are mSize*Time columns (see ?extract.obs) boot.R number of bootstrap samples boot.1 block size for blocked bootstrap t1 beginning of fit range t2 end of fit range parlist array of parameter combinations for the matrix fit vector of strings indicating the functional form of correlation functions which sym.vec were fitted RNG seed for bootstrap procedure seed mode1 see input. fit.method see input.

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

C. Michael, hep-lat/9412087hep-lat/9412087

See Also

```
cf, bootstrap.cf
```

Examples

reference_time The GEVP reference time for the principal correlator model

matrixModel 115

|--|

Description

Correlator matrix model.

Usage

```
matrixModel(par, t, Time, parind, sign.vec, ov.sign.vec, deltat = 0)
```

Arguments

par Numeric vector: Fit parameters of the model. In an object of type matrixfit,

this should be located at \$opt.res\$par.

t integer vector: Time of interest.Time integer: Time extent of the lattice.

parind See matrixfit.

sign.vec Numeric vector: Relative sign between forward and backwards propagating part.

A plus makes it cosh, a minus makes it sinh.

ov.sign.vec Numeric vector: Overal sign.

deltat Numeric: time shift.

Value

Returns a numeric vector with the same length as the input vector t containing the model evaluation for these t-values.

See Also

matrixfit

mom_combinations Generate table of momentum component combinations

Description

Generate table of momentum component combinations

Usage

```
mom_combinations(psqmax)
```

116 mul.raw_cf

Arguments

psqmax

Integer, maximum $p^2 = px^2 + py^2 + pz^2$ to be included in momentum list

Value

Returns a data.frame with all possible momentum combinations.

mul.cf

Arithmetically scale a correlator by a scalar a

Description

Note that this function is fundamentally different from *.cf.

Usage

```
mul.cf(cf, a = 1)
```

Arguments

cf cf_orig objects.

a Numeric, scaling factor.

Value

Returns an object of class cf.

mul.raw_cf

scale raw_cf data

Description

```
scale raw_cf data
```

Usage

```
mul.raw_cf(cf, a = 1)
```

Arguments

cf 'raw_cf' container with data to be scaled by the factor a

a Numeric or complex scaling factor, although it could also be an array of dimen-

sions compatible with cf\$data

Value

raw_cf object with res\$data == a*cf\$data

new_matrixfit 117

| new_matrixfit | perform a factorising fit of a matrix of correlation functions |
|---------------|--|
| | |

Description

Modernised and extended implementation of matrixfit

Usage

```
new_matrixfit(cf, t1, t2, parlist, sym.vec = rep(1, cf$nrObs),
  neg.vec = rep("cosh", cf$nrObs), useCov = FALSE, model = "single",
  boot.fit = TRUE, fit.method = "optim", autoproceed = FALSE, par.guess,
  every, higher_states = list(val = numeric(0), boot = matrix(nrow = 0, ncol
  = 0), ampl = numeric(0)), ...)
```

Arguments

| cf | Object of class cf with cf_meta and cf_boot. |
|---------------|---|
| t1 | Integer, start time slice of fit range (inclusive). |
| t2 | Integer, end time slie of fit range (inclusive). |
| parlist | Numeric vector, list of parameters for the model function. |
| sym.vec | Integer, numeric or vectors thereof specifying the symmetry properties of the correlation functions stored in cf. See matrixfit for details. |
| neg.vec | Integer or integer vector of global signs, see matrixfit for details. |
| useCov | Boolean, specifies whether a correlated chi^2 fit should be performed. |
| model | String, specifies the type of model to be assumed for the correlator. See below for details. |
| boot.fit | Boolean, specifies if the fit should be bootstrapped. |
| fit.method | String, specifies which minimizer should be used. See matrixfit for details. |
| autoproceed | Boolean, if TRUE, specifies that if inversion of the covariance matrix fails, the function should proceed anyway assuming no correlation (diagonal covariance matrix). |
| par.guess | Numeric vector, initial values for the paramters, should be of the same length as parlist. |
| every | Integer, specifies a stride length by which the fit range should be sparsened, using just everyth time slice in the fit. |
| higher_states | List with elements val and boot. Only used in the n_particles fit model. The member val must have the central energy values for all the states that are to be fitted. The boot member will be a matrix that has the various states as columns and the corresponding bootstrap samples as rows. The length of val must be the column number of boot. The row number of boot must be the number of samples. |
| • • • | Further parameters. |

new_matrixfit

Details

There are different fit models available. The models generally depend on one or multiple energies E and amplitudes p_i which for a general matrix are row- and column-amplitudes. The relative sign factor $c \in \{-1, 0, +1\}$ depends on the chosen symmetry of the correlator. It is a plus for a "cosh" symmetry and a minus for a "sinh" symmetry. If the back propagating part is to be neglected (just "exp" model), it will be zero.

When the back propagating part is not taken into account, then the single, shifted and weighted model become the same except for changes in the amplitude.

• single: The default model for a single state correlator is

$$\frac{1}{2}p_i p_j(\exp(-p_1 t) \pm c \exp(-p_2 (T-t))).$$

• shifted: If the correlator has been shifted (using takeTimeDiff.cf, then the following model is applicable:

$$p_i p_i (\exp(-p_1(t+1/2)) \mp c \exp(-p_1(T-(t+1/2))))$$
.

- weighted: Works similarly to the shifted model but includes the effect of the weight factor from removeTemporal.cf.
- pc: In case only a single principal correlator from a GEVP is to be fitted this model can be used. It implements

$$\exp(-p_1(t-t_0))(p_2+(1-p_2)\exp(-p_3(t-t_0))$$

with t_0 the reference timesclice of the GEVP. See bootstrap.gevp for details.

• two_amplitudes: Should there be a single state but different amplitudes in the forward and backwards part, the following method is applicable.

$$\frac{1}{2}(p_2 \exp(-p_1 t) \pm c p_3 \exp(p_1 t))$$

This only works with a single correlator at the moment.

• single_constant: Uses the single model and simply adds $+p_3$ to the model such that a constant offset can be fitted. In total the model is

$$single(p_1, p_2) + p_3$$
.

• n_particles: A sum of single models with independent energies and amplitudes:

$$\sum_{i=1}^{n} \operatorname{single}(p_{2n-1}, p_{2n}).$$

Use the higher_states parameter to restrict the thermal states with priors to stabilize the fit.

Value

See bootstrap.nlsfit.

old_removeTemporal.cf Remove temporal states

Description

Performs weighting and shifting in the rest and moving frames.

Usage

```
old_removeTemporal.cf(cf, single.cf1, single.cf2, p1 = c(0, 0, 0), p2 = c(0, 0, 0), L, lat.disp = TRUE, weight.cosh = FALSE, deltat = 1)
```

Arguments

Object of type cf, two-to-two particle correlation function which shall be weighted and shifted. It must be a correlation function in the frame $p_1 + p_2$.

single.cf1, single.cf2

Object of type effectivemassfit or matrixfit which contains the one particle mass in the rest frame.

If single.cf2 is missing, then the mass given as single.cf1 is used as well. This is sensibly done when one scatters identical particles. But be careful: Even when single.cf2 is missing, the p2 is *not* automatically copied from p1.

In case single.cf1 is missing, no weighting is performed. Instead it is assumed that the user only wants to have a simple shifting. Then this function just calls takeTimeDiff.cf.

p1, p2 Integer vector with three elements, containing the momenta that the one particle mass should be boosted to.

Integer, spatial extent of the lattice.

lat.disp Logical, true when the lattice dispersion relation shall be used, otherwise con-

tinuum dispersion relation.

weight.cosh Logical, If single.cfl is a pure cosh, the leading two thermal states also may be

expressed as a cosh. If weight.cosh is set, they are removed simultaneously.

deltat Integer. Time shift value.

Value

Returns an object of class cf, see cf.

onlinemeas

| onlinemeas | determines pion mass and pcac mass from online measured correlator of the HMC code |
|------------|--|
| | · |

Description

determines pion mass and pcac mass from online measured correlator of the HMC code

Usage

```
onlinemeas(data, t1, t2, stat_range, S = 1.5, pl = FALSE, skip = 0,
iobs = 1, ind.vec = c(1, 3, 4, 5), mu = 0.1, kappa = 0.125,
boot.R = 99, boot.l = 10, tsboot.sim = "geom", method = "uwerr",
fit.routine = "optim", nrep, oldnorm = FALSE)
```

Arguments

| data | data to be fitted to as e.g. the output of readcmicor. Currently only cmicor format is supported. | | | |
|------------|---|--|--|--|
| t1 | lower bound for the fitrange in time (t1,t2). Counting starts with 0. | | | |
| t2 | upper bound for the fitrange in time (t1,t2). Counting starts with 0. | | | |
| stat_range | range of data to be included in the analysis. | | | |
| S | passed to uwerr, see documentation of uwerr. | | | |
| pl | logical: if set to TRUE the function produces plots | | | |
| skip | number of measurements to be discarded at the beginning of the time series. skip has no effect if two or more replica are used, see argument nrep. | | | |
| iobs | if there are several operators available (local-local, local-smeared, etc.), then this labels these (for cmi format) | | | |
| ind.vec | index vector indexing the column numbers in cmicor to be used | | | |
| mu | twisted mass parameter. | | | |
| kappa | hopping parameter. | | | |
| boot.R | number of bootstrap samples for bootstrap analysis | | | |
| boot.1 | average block size for blocking analysis with tsboot | | | |
| tsboot.sim | The type of simulation required to generate the replicate time series. See tsboot for details. | | | |
| method | the type of error analysis to be used. Can be either "uwerr", "boot", "all" or "no". For "no" (or any other string) no error analysis is performed. This might be helpful for a first impression and also to test different initial values for the fitting parameters. The latter is in particular needed for more than one state in the fit. | | | |

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fit.routine The fit routine to be used. Default is "gsl", which uses the gnu scientific library

"gsl_multifit_fdfsolver" solver to minimise the chisquare. All other values lead to the usage of R's optim function. The latter choice might be significantly

slower.

nrep vector (N1, N2, ...) of replica length N1, N2. If missing it is assumed that there

is only one ensemble. If there are two or more replica the parameter skip has

no effect.

oldnorm If set to "TRUE", the old online measurement normalisation of "tmLQCD" prior

to version 5.2.0 is used in order to get correct values for the pion decay constant.

Details

The online measurements in the HMC code compute the PP and PA correlation functions summed over spatial x for all t. We analyse these correlators in different ways:

First, only the PP correlator is analysed and fitted by $p_1^2 \cosh(-m(t-T/2))$ for m and p_1 .

Second, PP and PA correlators are fitted together with three parameters as $C_{\rm PP}=p_1^2\cosh(-m(t-T/2))$ and $C_{\rm PA}=p_1p_2\cosh(-m(t-T/2))$ in a simultaneous fit. m is then the pseudo scalar mass and the pcac mass is determined from

$$m_{\rm PCAC} = m_{\rm PS} \frac{p_2}{2p_1}$$

Finally, the PCAC mass can also be determined computing

$$m_{\mathrm{PCAC}}(t) = \frac{C_{\mathrm{PA}}(t+1) - C_{\mathrm{PA}}(t-1)}{4C_{\mathrm{PP}}(t)}$$

using the symmetric finite difference operator.

Value

returns an object of class of it with the following items

fitresult result from the fit as returned by optim

fitresultpp Fit result of the PP correlator only

t1 lower bound for the fitrange in time (t1,t2). Counting starts with 0. t2 upper bound for the fitrange in time (t1,t2). Counting starts with 0.

N number of measurements found in the data

Time Time extent found in the data

fitdata data.frame containing the time values used in the fit, the averaged correlator

and its error and the value of Chi for each time value

uwerrresultmps the result of the time series analysis for the lowest mass as carried out by uwerr uwerrresultmpcac

the result of the time series analysis for the PCAC mass carried out by uwerr,

see details

effmass effective masses in the pion channel

matrix.size size of the data matrix, copied from input

boot object returned by the call to boot if method was set correspondingly. Otherwise

NULL.

tsboot object returned by the call to tsboot if method was set correspodingly. Other-

wise NULL.

method error analysis method as copied from input

fit.routine fit.routine as copied from input

nrep as copied from input

dpaopp data.frame containing the peac masses computed not with a fit, but with the

derivative method for all time values in between t1 and t2

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readcmicor, uwerr,
```

overview_plot_raw_cf create convenient overview plots for a raw_cf object

Description

create convenient overview plots for a raw_cf object

Usage

```
overview_plot_raw_cf(cf, grid, reim = "real", reim_same = FALSE,
  relerr = FALSE, tauint = FALSE, value_logplot = TRUE,
  value_factor = c(1), title = "")
```

Arguments

| cf | 'raw_ | cf' | container | with | data | and | meta-da | ta |
|----|-------|-----|-----------|------|------|-----|---------|----|
|----|-------|-----|-----------|------|------|-----|---------|----|

grid Optional, integer vector which satisfies prod(grid) == prod(cf\$dim). This is

passed to par via par(mfrow=grid) to produce a grid of plots as defined by the

components of grid.

reim Vector of strings, one of 'real', 'imag' or 'both'. Specified whether the real or

imaginary parts (or both) should be plotted.

reim_same Boolean, whether real and imaginary parts should be plotted on the same plot.

If TRUE, then reim must be 'both'. If this is given, the imaginary part as well as

its relative error and per-time-slice integrated autocorreation times

relerr Boolean, whether a plot of the relative error per time slice should be added.

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tauint Boolean, whether a plot of the integrated auto-correlation time on each time

slice should be added.

value_logplot Boolean, whether the plot of the correlator should be on a logarithmic vertical

axis. (does not affect tauint and relerr).

value_factor Numeric, either of length '1' or as long as the number of correlation functions

in cf. The data will be scaled by this factor before plotting.

title Character vector, will be passed as the main argument to plotwitherror which in

turn passes it to plot. Can be either of length '1' or prod(cf\$dim)

Value

No return value, only plots are generated.

parametric.bootstrap Parametric bootstrap

Description

Parametric bootstrap

Usage

```
parametric.bootstrap(boot.R, x, dx, seed)
```

Arguments

boot .R numeric. Number of bootstrap samples to generate.

x numeric vector. Actual values for the data.

dx numeric vector of the same length as x or missing. Errors of the values.

seed integer. Seed to use for the random number generation. If it is missing, the seed

will not be set to any particular value. If there was a default value, all results would be exactly correlated. So if you want reproducability by fixing the seeds,

make sure you choose different seeds for independent variables.

Value

A matrix with as many columns as there are variables in x and as many rows as boot.R.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

Examples

```
x <- 1:3

dx <- 1:3 * 0.1

parametric.bootstrap(5, x, dx)
```

parametric.bootstrap.cov

Parametric bootstrap with covariance

Description

Parametric bootstrap with covariance

Usage

```
parametric.bootstrap.cov(boot.R, x, cov, seed)
```

Arguments

boot.R numeric. Number of bootstrap samples to generate.

x numeric vector. Actual values for the data.

cov numeric matrix, square, length of x or missing. Covariance between the various

variables in the vector x.

seed integer. Seed to use for the random number generation. If it is missing, the seed

will not be set to any particular value. If there was a default value, all results would be exactly correlated. So if you want reproducability by fixing the seeds,

make sure you choose different seeds for independent variables.

Value

A matrix with as many columns as there are variables in x and as many rows as boot. R.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.nlsfit(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

Examples

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| parametric.nlsfit | NLS | fit with parametric bootstrap |
|-------------------|-----|-------------------------------|
| | | |

Description

NLS fit with parametric bootstrap

Usage

```
parametric.nlsfit(fn, par.guess, boot.R, y, dy, x, dx, lower = rep(x = -Inf,
  times = length(par.guess)), upper = rep(x = +Inf, times =
  length(par.guess)), ..., bootstrap = TRUE)
```

Arguments

| fn | fn(par, x,). The (non-linear) function to be fitted to the data. Its first argument must be the fit parameters named par. The second must be x, the explaining variable. Additional parameters might be passed to the function. Currently we pass boot.r which is 0 for the original data and the ID $(1,)$ of the bootstrap sample otherwise. As more parameters might be added in the future it is recommended that the fit function accepts as the last parameter to be forward compatible. |
|-----------|--|
| par.guess | initial guess values for the fit parameters. |
| boot.R | numeric. Number of bootstrap samples to generate. |
| У | the data as a one-dimensional numerical vector to be described by the fit function. |
| dy, dx | Numeric vector. Errors of the dependent and independent variable, respectively. These do not need to be specified as they can be computed from the bootstrap samples. In the case of parametric bootstrap it might would lead to a loss of information if they were computed from the pseudo-bootstrap samples. They must not be specified if a covariance matrix is given. |
| X | values of the explaining variable in form of a one-dimensional numerical vector. |
| lower | Numeric vector of length length(par.guess) of lower bounds on the fit parameters. If missing, -Inf will be set for all. |
| upper | Numeric vector of length length(par.guess) of upper bounds on the fit parameters. If missing, +Inf will be set for all. |
| | Additional parameters passed to fn, gr and dfn. |
| bootstrap | Shall the error calculation be performed using boostrap? If not, the errors are estimated with help of the jacobian (either provided in gr or calculated using the numDeriv-package). |

Value

See simple.nlsfit.

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See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

Examples

```
## Declare some data. value <- c(0.1, 0.2, 0.3) dvalue <- c(0.01, 0.01, 0.015) x <- c(1, 2, 3) dx <- c(0.1, 0.1, 0.1) boot.R <- 1500 fn <- function (par, x, ...) par[1] + par[2] * x fit.result <- parametric.nlsfit(fn, c(1, 1), boot.R, value, dvalue, x, dx) summary(fit.result)
```

parametric.nlsfit.cov

Description

NLS fit with parametric bootstrap and covariance

Usage

```
parametric.nlsfit.cov(fn, par.guess, boot.R, y, x, cov, lower = rep(x = -Inf, times = length(par.guess)), upper = rep(x = +Inf, times = length(par.guess)), ..., bootstrap = TRUE, na.rm = FALSE)
```

Arguments

| fn | fn(par, x,). The (non-linear) function to be fitted to the data. Its first argument must be the fit parameters named par. The second must be x, the explaining variable. Additional parameters might be passed to the function. Currently we pass boot.r which is 0 for the original data and the ID (1,) of the bootstrap sample otherwise. As more parameters might be added in the future it is recommended that the fit function accepts as the last parameter to be forward compatible. |
|-----------|--|
| par.guess | initial guess values for the fit parameters. |
| boot.R | numeric. Number of bootstrap samples to generate. |
| У | the data as a one-dimensional numerical vector to be described by the fit function. |
| X | values of the explaining variable in form of a one-dimensional numerical vector. |

pcac 127

| cov | numeric matrix, square, length of x or missing. Covariance between the various variables in the vector x . |
|-----------|---|
| lower | Numeric vector of length length(par.guess) of lower bounds on the fit parameters. If missing, -Inf will be set for all. |
| upper | Numeric vector of length length(par.guess) of upper bounds on the fit parameters. If missing, +Inf will be set for all. |
| | Additional parameters passed to fn, gr and dfn. |
| bootstrap | boolean. If TRUE, bootstrap is used. |
| na.rm | logical. If set to true, NAs in y and dy will be ignored. If x-errors are taken into account, NAs in x and dx will be ignored, too. |

Value

See simple.nlsfit.

See Also

Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()

pcac Computes the pcac mass

Description

Computes the pcac mass from the PP and the AP (PA) correlators and estimates the errors using the gamma method

Usage

```
pcac(psfilename, apfilename, pafilename, from = 3, to = 3, fit = F, skip = 0, plotit = F, S = 1.5)
```

Arguments

| psfilename | filename of the file from which to read the PP correlator. It is supposed to be in GWC code format. mandatory. |
|------------|--|
| apfilename | filename of the file from which to read the AP correlator. It is supposed to be in GWC code format. Either PA or AP correlator (or both) must be given. If both are given, both are used by averaging. |
| pafilename | filename of the file from which to read the PA correlator. It is supposed to be in GWC code format. Either PA or AP correlator (or both) must be given. If both are given, both are used by averaging. |
| from | the effective mass is computed starting with t=from |

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| to | the effective mass is computed ending with t=to |
|--------|---|
| fit | logical. if TRUE a fit is performed to all t-values to determine the pcac mass. |
| skip | no of measurements to skip at the beginning of the file |
| plotit | logical. if TRUE a plot is drawn. |
| S | passed to uwerr, see documentation of uwerr. |

Details

the symmetric difference operator is used.

Value

returns a data.frame with the results. The object is also of class massfit which can be plotted using the generic function plot.

Author(s)

Carsten Urbach, <carsten.urbach@liverpool.ac.uk>

|--|--|

Description

Computes the average PCAC mass

Usage

```
pcacfit(data, from, to, T2, pa = FALSE)
```

Arguments

| data | 'Effectivemasses' from correlators |
|------|------------------------------------|
| from | initial value of fit range |
| to | final value of fit range |
| T2 | Time extent |
| ра | Boolean. |

Value

Single numeric value, the mass.

pcModel 129

| | | | | | _ |
|----|---|--------|---|--------|---|
| pc | v | \sim | А | \sim | |
| DC | ľ | U | u | c | 1 |

Principal correlator two state model.

Description

Principal correlator two state model.

Usage

```
pcModel(par, t, Time, delta1 = 1, reference_time)
```

Arguments

par Numeric vector: Fit parameters of the model. In an object of type matrixfit,

this should be located at \$opt.res\$par.

t Numeric vector: Time of interest.Time Numeric: Time extent of the lattice.

delta1 dummy parameter for compatibility

reference_time Numeric: GEVP reference time value in physical time convention

Value

Returns a numeric vector with the same length as the input vector t containing the model evaluation for these t-values.

See Also

matrixfit

pgevm2bootstrapfit

pgevm2bootstrapfit

Description

```
pgevm2bootstrapfit
```

Usage

```
pgevm2bootstrapfit(pgevm, truncation.dim = pgevm$opt.idx[1],
  errortype = "outlier-removal")
```

130 pgevm2effectivemass

Arguments

pgevm an object of class 'PGEVM' generated by 'bootstrap.truncated.pgevm'

truncation.dim integer. The truncation dimension to be used. Default is the most likely optimal

truncation dimension pgevm\$opt.idx.

errortype string. Determines the treatment of the bootstrap histograms to determine the

statistical error on fit result. Can be: 1. 'outlier-removal' for which outliers are removed according to the 0.25 and 0.75 quantiles and the inter-quantile-range, i.e. only values are kept which are in the interval $[Q_25-1.5IQR,Q_75+1.5IQR]$ and the error is computed from the standard deviation of the bootstrap distribution. 2. 'std-dev' for which the error is estimated from the standard

deviation.

Value

Returns an object of S3 class bootstrapfit.

See Also

input is generated via bootstrap.truncated.pgevm See also bootstrap.nlsfit

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2effectivemass(), plot_hankel_spectrum()

pgevm2effectivemass pgevm2effectivemass

Description

pgevm2effectivemass

Usage

```
pgevm2effectivemass(pgevm, id = c(1), type = "log", eps = 1e-16, n.max,
probs = c(0.16, 0.84), errortype = "outlier-removal",
bias_correction = FALSE, average.negE = FALSE, range = c(0.1, 1))
```

Arguments

| pgevm | an object of class 'PGEVM' generated by 'bootstrap.pgevm' or 'bootstrap.truncated.pgevm' |
|-------|--|
| id | integer. The id of the state to be determined |
| type | Character vector. Type of effective mass to use. Must be in c("log") |
| eps | numeric. threshold for zero |
| n.max | integer. The maximal value of 'n' to consider |
| probs | numeric. The probabilities for errortype quantiles, default is c(0.16,0.84). |

plaq.sample 131

errortype

string. Determines the treatment of the bootstrap histograms to determine the statistical error on eigenvalues. Can be: 1. 'outlier-removal' for which outliers are removed according to the 0.25 and 0.75 quantiles and the inter-quantile-range, i.e. only values are kept which are in the interval $[Q_25-1.5IQR,Q_75+1.5IQR]$ and the error is computed from the standard deviation of the bootstrap distribution. 2. 'quantiles' for which the error is estimated from the difference between the 0.32 and 0.68 quantile of the original bootstrap distribution 3. 'db-boot' which works only, if the 'cf' is double bootstrapped. It will estimate the error from the true error of the median

bias_correction

boolean. If set to 'TRUE', the median of the bootstrap distribution is used as

estimator for the energy values.

average.negE boolean. If set to TRUE average over positive and negative energies

range numeric. Range of eigenvalues to consider for the effective mass.

Value

Returns an object of S3 class effectivemass.

See Also

input is generated via bootstrap.pgevm or bootstrap.truncated.pgevm. See also bootstrap.effectivemass

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), plot_hankel_spectrum()

plaq.sample

Sample plaquette time series

Description

A time series of so-called plaquette values generated by a Markov Chain MC process using the Hybrid Monte-Carlo algorithm. Plaquettes are the smallest possible closed loops which can be build in lattice QCD in discretised Euclidean space time.

Format

The format is: num 0.583 0.582 0.582 0.582 0.582 ...

Examples

```
data(plaq.sample)
plot(x=c(1:length(plaq.sample)), y=plaq.sample, type="1", xlab="t", ylab="<P>")
```

plot.bootstrapfit

plot.averx

Plots averx data

Description

Plots averx data

Usage

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

Arguments

x averx object ignored

Value

Returns the plotted data in from of a data.frame with named columns t (the time index), averx the values of average x and daverx the statistical error estimate.

plot.bootstrapfit

Plot a bootstrap NLS fit

Description

Plot a bootstrap NLS fit

Usage

```
## S3 method for class 'bootstrapfit'
plot(x, ..., col.line = "black", col.band = "gray",
  opacity.band = 0.65, lty = c(1), lwd = c(1), supports = 1000,
  plot.range, error = x$error.function, ribbon.on.top = TRUE,
  rep = FALSE)
```

Arguments

x object returned by bootstrap.nlsfit

... Additional parameters passed to the plotwitherror function.

col.line line colour.

col.band error band colour.
opacity.band error band opacity.

plot.cf 133

line type of fitted curve. 1ty line width for fitted curve. lwd supports number of supporting points for plotting the function. vector with two elements c(min, max) defining the range in which fitline and plot.range errorband are plotted. Default is the range of the data. Function to compute the standard error in resampling schemes. Default is sd for error bootstrap. For other resampling schemes this might need to be changed. Logical, controls whether the ribbon should be in front of the data points. This ribbon.on.top is recommended when there are very many data points and a highly constrained model. rep

If set to TRUE, operate like "replot" in gnuplot. Allows plotting the fit result on top of existing plot.

Value

No return value.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

plot.cf

Plot a correlation function

Description

Plot a correlation function

Usage

```
## S3 method for class 'cf'
plot(x, neg.vec = rep(1, times = length(x$cf0)), rep = FALSE,
    ...)
```

Arguments

x cf_boot object

neg.vec Numeric vector of length cf\$cf0. This allows switching the sign for certain time slices or observables such that displaying in log-scale is sensible.

rep See plotwitherror.

... Graphical parameter to be passed on to plotwitherror

plot.coshfit

Value

Invisibly returns a data.frame with named columns t containing the (physical) t-values, CF the mean values of the correlation function and Err its standard error.

plot.cfit

plot.c1fit

Description

Generic function to plot an object of type c1fit

Usage

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

Arguments

x Object of type c1fit

... Generic graphical parameter to be passed on to plotwitherror

Value

No return value, only plots are generated.

plot.coshfit

Plot a cosh-fit

Description

Plot a cosh-fit

Usage

```
## $3 method for class 'coshfit'
plot(x, col.fitline = "black", plot.mass = TRUE,
    plot.corr = FALSE, ...)
```

Arguments

x An object generated by fit.cosh. col.fitline Color in which the fit is visualized. plot.mass, plot.corr

The plot can show the fitted correlator (plot.corr) as well as the corresponding effective mass (plot.mass, if fitted with effMass).

... graphical parameters to be passed on to plotwitherror

plot.effectivemass 135

Value

No return value.

plot.effectivemass

plot.effectivemass

Description

plot.effectivemass

Usage

```
## S3 method for class 'effectivemass'
plot(x, ..., ref.value, col, col.fitline, xshift = 0)
```

Arguments

x Object of class effectivemass

... Graphical parameters to be passed on to plotwitherror

ref.value Numeric. A reference value to be plotted as a horizontal line

col String. Colour of the data points.col.fitline String. Colour of the fitted line.

xshift Numeric. Shift to be applied to the x-values.

Value

No return value.

plot.effmass

plot.effmass

Description

```
plot.effmass
```

Usage

```
## S3 method for class 'effmass'
plot(x, ..., 11, 1f, ff)
```

plot.gevp.amplitude

Arguments

| X | Object of class effmass |
|-------|---------------------------------------|
| • • • | Graphical parameters to be passed on. |
| 11 | local-local effective mass object |
| lf | local-fuzzed effective mass object |
| ff | fuzzed-fuzzed effective mass object |

Value

No value returned, only plots are generated.

```
plot.gevp.amplitude plot.gevp.amplitude
```

Description

plot.gevp.amplitude

Usage

```
## S3 method for class 'gevp.amplitude'
plot(x, xlab = "t", ylab = paste0("P[,", x$id,
   ",", x$op.id, "]"), ...)
```

Arguments

| X | Object of type gevp.amplitude. |
|------|--------------------------------------|
| xlab | x axis label |
| ylab | y axis label |
| | Graphical parameters to be passed on |

Value

No return value.

plot.hadronacf 137

plot.hadronacf

Description

generic function to plot an object of class "myGamma"

Usage

```
## S3 method for class 'hadronacf'
plot(x, ..., col = "black")
```

Arguments

x Object of type hadronacf generated by computeacf
 ... Generic graphical parameters to be passed on
 col String. Color to be used for the data points.

Value

No return value.

plot.massfit plot.massfit

Description

Generic function to plot an object of type massfit

Usage

```
## S3 method for class 'massfit'
plot(x, ..., xlab = "t", ylab = "m")
```

Arguments

| X | Object of type massfit |
|------|--|
| | Generic graphical parameter to be passed on to plotwitherror |
| xlab | String. Label for x-axis |
| ylab | String. Lable for y-axis |

Value

See plotwitherror.

plot.matrixfit

|--|

Description

Plot a matrixfit

Usage

```
## S3 method for class 'matrixfit'
plot(x, plot.errorband = FALSE, ylim, xlab = "t/a",
  ylab = "y", do.qqplot = TRUE, plot.raw = TRUE, rep = FALSE, col,
  every, ...)
```

Arguments

| X | an object of class matrixfit |
|----------------|--|
| plot.errorband | Boolean: whether or not to plot an errorband |
| ylim | Numeric vector: y-limit of the plot |
| xlab | String: label of x-axis |
| ylab | String: label of y-axis |
| do.qqplot | Boolean: whether or not to plot an QQ-plot |
| plot.raw | Boolean: plot the raw data or multiply out the leading exponetial behaviour |
| rep | Boolean: whether or not to add to existing plot |
| col | String vector: vector of colours for the different correlation functions |
| every | Fit only a part of the data points. Indices that are not multiples of every are skipped. If no value is provided, all points are taken into account. |
| | Graphical parameters to be passed on to plot or plotwitherror. |

Value

Returns no value, generated only plots.

See Also

```
matrixfit
```

plot.ofit 139

plot.ofit

plot.ofit

Description

Generic function to plot an object of type of it

Usage

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

Arguments

x Object of type of it

... Generic graphical parameter to be passed on to plotwitherror

Value

See plot.cfit

plot.outputdata

Plot Command For Class Ouputdata

Description

Generic plot routine for class "ouputdata". Currently it plots the plaquette history and the history of ΔH

Usage

```
## S3 method for class 'outputdata'
plot(x, skip = 0, ...)
```

Arguments

x object of class "outputdata" obtained from a read with readoutputdata skip number of trajectories to be skipped in analysis for plaquette and $\exp(-\Delta H)$ additional arguments passed to the generic plot function.

plot.pionff

Value

list containing the "data", an object of class "uwerr" called "plaq.res" containing the statistical analysis for the plaquette and a second object of type "uwerr" called "dH.res" with the statistical analysis for $\exp(-\Delta H)$.

The plotted data is return in form of a list with named elements data containing the input data, plaq.res an object returned by uwerrprimary for the plaquette data dn dH. res an object returned by uwerrprimary for ΔH .

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
readoutputdata, uwerr
```

Examples

```
plaq <- readoutputdata(paste0(system.file(package="hadron"), "/extdata/output.data"))
plaq.plot <- plot(plaq, skip=100)
summary(plaq.plot$plaq.res)</pre>
```

plot.pionff

plot.pionff

Description

Generic function to plot an object of type pionff

Usage

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

Arguments

x Object of type pionff

... Generic graphical parameter to be passed on to plotwitherror

Value

No return value, only plots are generated.

plot.raw_cf

plot.raw_cf

plot all correlators in raw_cf object

Description

plot all correlators in raw_cf object

Usage

```
## S3 method for class 'raw_cf'
plot(x, ..., reim = "real", reim_same = FALSE)
```

Arguments

x Object of class raw_cf with data and meta-data.

... Further parameters passed to plotwitherror.

reim Character vector, may contain 'real', 'imag' or 'both'. Determines whether the

real and/or imaginary parts of the correlation funtions should be plotted.

reim_same Boolean, determines whether the real and imaginary parts, if both are to be

plotted, will be plotted in the same plot.

Value

Invisibly returns the plotdata, see get_plotdata_raw_cf.

```
plot.truncated.pgevm plot.truncated.pgevm
```

Description

plot.truncated.pgevm

Usage

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

Arguments

x Object of type truncated.pgevm.

... Graphical parameters to be passed on.

Value

No return value.

142 plot.uwerr

| | p | 1 | 0 | t | | uwe | rr | _ |
|--|---|---|---|---|--|-----|----|---|
|--|---|---|---|---|--|-----|----|---|

Plot Command For Class UWerr

Description

Plot Command For Class UWerr

Usage

```
## S3 method for class 'uwerr'
plot(x, ..., main = "x", plot.hist = TRUE, index = 1,
    Lambda = 100)
```

Arguments

| Χ | object of class uwer |
|---|----------------------|
| X | object of class uwer |

... generic parameters, not used here.

main main title of the plots.

plot.hist whether or not to generate a histogram

index index of the observable to plot.

Lambda Cutoff to be used in the error computation for the ACF.

Value

produces various plots, including a histogram, the autocorrelation function and the integrated autocorrelation time, all with error bars.

No return value.

Author(s)

Carsten Urbach, <carsten.urbach@liverpool.ac.uk>

See Also

uwerr

Examples

```
data(plaq.sample)
plaq.res <- uwerrprimary(plaq.sample)
plot(plaq.res)</pre>
```

plothlinewitherror 143

ploth line with error

Description

plot a horizontal line with error band

Usage

```
plothlinewitherror(m, dp, dm, col = c("red"), x0, x1)
```

Arguments

| m | Numeric. Mean value of the line to plot. |
|-----|---|
| dp | Numeric. Error up. |
| dm | Numeric. Error down. |
| col | String. Colour. |
| x0 | Numeric. Left value of the range of the horizontal line. |
| x1 | Numeric. Right value of the range of the horizontal line. |

Value

No return value, only graphics is generated.

| plot | : - | +ha | | |
|------|------------|-----|-----|---|
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Plot Command For XY Plots With Error Bars

Description

Plot command for XY scatterplots based on plot and points which provides support for multiple, non-symmetric error bars. Error bars are drawn as vertical or horizontal lines originating from the point with narrow, perpendicular lines at the end of the error bar (end caps). When multiple errors are drawn, the width of the perpendicular line increases from the innermost error bar to the outermost one. Different summation methods for the individual errors are supported.

Usage

```
plotwitherror(x, y, dy, ylim = NULL, dx, xlim = NULL, mdx, mdy,
  errsum.method = "linear.quadrature", rep = FALSE, col = "black", ...)
```

Arguments

x vector of x coordinatesy vector of y coordinates

dy one of:

- Vector of errors on y coordinates.
- Array, matrix or data frame if multiple error bars are to be drawn, such that each column refers to one error. The individual errors should be provided as is, because they are summed internally to draw the final error bars. A given column can also be provided with 0 entries, in which case the error bar will be drawn, but it will have zero length, such that only the end caps for this error will be visible.

ylim limits for y-axis

dx Same as dy, but for the x coordinate.

xlim limits for x-axis

mdx Support for non-symmetric error bars. Same as dx, but for errors in the negative

x-direction. Errors should be provided as positive numbers, the correct sign will

be added internally. If not provided, dx is used as a symmetric error.

mdy Same as mdx but for the y coordinate.

errsum.method Determines how the invidual errors should be summed for display purposes.

Valid argument values are:

- "linear"
 - Individual errors are summed linearly, such that the distance from the point to the i'th error bar, l_i , is

$$l_i = \sum_{j=1}^i e_j$$

Hence, the third error bar, for example, would be located at

$$l_3 = e_1 + e_2 + e_3$$

while the second error bar is at

$$l_2 = e_1 + e_2$$

- "quadrature"
 - Individual errors are summed in quadrature and error bars are drawn at the fractional position according to the following formula:

$$l_{max} = \sqrt{\sum_{j=1}^{max} e_j^2}$$

$$l_i = \sum_{j=1}^{i} e_j^2 / l_{max}$$

- "linear.quadrature"
 - Errors are summed as for "linear", but the total error summed in quadrature is also indicated as an end cap of triple line width

rep If set to TRUE, operate like "replot" in gnuplot. Allows adding points with error bars to the current plot. Switches the underlying plotting routine from plot to

points.

col colour of plotted data

... any graphic options passed over to plot

Value

a plot with error bars is drawn on the current device

Returns for convenience a list with elements xlim and ylim representing the x- and y-limits chosen by the routine.

Author(s)

```
Carsten Urbach, <urbach@hiskp.uni-bonn.de>
Bartosz Kostrzewa, <bartosz.kostrzewa@desy.de>
```

See Also

```
plot, points
```

Examples

```
# Create some random data, set one error to zero. x <-1:50 y <- runif(50, 0, 1) dy <- runif(50, 0.1, 0.2) dy[4] <- 0 plotwitherror(x, y, dy)
```

Description

function to plot timeseries of eigenvlues, including minimum and maximum eigenvalue bands as found in the monomial_0x.data files produced by tmLQCD

Usage

```
plot_eigenvalue_timeseries(dat, stat_range, ylab, plotsize, filelabel,
  titletext, pdf.filename, errorband_color = rgb(0.6, 0, 0, 0.6),
  debug = FALSE)
```

Arguments

dat Timeseries to analyse. stat_range range of statistics to use.

ylab Y-axis label.

plotsize Width and Height of plot.

filelabel String. Label of the file.

titletext Text in the plot title.

pdf.filename String. PDF filename.

errorband_color

String. Colour of the error band.

debug Boolean. Generate debug output.

Value

Returns a list with two named elements mineval and maxeval for the minimal and the maximal eigenvalue, see plot_timeseries.

```
plot_hankel_spectrum plot_hankel_spectrum
```

Description

produces a scatter plot of the complex $-\log$ of the eigenvalues produced by the bootstrap.hankel method. In addition, produces a histogramm of all real and positive eigenvalues after computing $-\log(ev)/\delta t$ in the range (0,1) and determines its mode.

Usage

```
plot_hankel_spectrum(hankel, deltat = 1, id = c(1:hankel$n))
```

Arguments

hankel object as returned from bootstrap.hankel deltat Integer. Time shift at which to plot

id Integer vector. Indices of eigenvalues to be plotted. Must be part of c(1:hankel\$n).

Value

No return value.

plot_timeseries 147

See Also

Other hankel: bootstrap.hankel(), bootstrap.hankel_summed(), bootstrap.pgevm(), bootstrap.truncated.pgevm gevp.hankel(), gevp.hankel_summed(), gevp.truncated.hankel(), hankel2cf(), hankel2effectivemass(), pgevm2bootstrapfit(), pgevm2effectivemass()

plot_timeseries plot_timeseries

Description

function to plot timeseries data, a corresponding histogram and an error shading for an error analysis via uwerr

Usage

```
plot_timeseries(dat, ylab, plotsize, titletext, hist.by, stat_range = c(1, length(dat$y)), pdf.filename, name = "", xlab = "$t_\\mathrm{MD}$", hist.probs = c(0, 1), errorband_color = rgb(0.6, 0, 0, 0.6), type = "1", uwerr.S = 2, smooth_density = FALSE, periodogram = FALSE, debug = FALSE, uw.summary = TRUE, ...)
```

Arguments

dat Timeseries to analyse.

ylab Y-axis label.

plotsize Width and Height of plot. titletext Text in the plot title.

hist.by Numeric. Stepping to compute the histogram breaks.

stat_range Optional integer vector of length 2. Start and end indices of the subset of dat to

be plotted. If left empty, all of dat will be plotted.

pdf.filename String. PDF filename.
name String. Timeseries name.

xlab X-axis label.

hist.probs Optional numeric vector of length 2. Probability extrema to limit the width of

the histogram or smoothed density plots. By default all data is used. Note: this

has not effect on the analysis as a whole or other plots.

errorband_color

String. Colour of the error band.

type String. Plot type, see plot for details.

uwerr. S Numeric. S of the uwerr method to be used.

smooth_density Boolean. Instead of plotting a histogram, use a smoothed density.

periodogram Boolean. Whether to show a periodogram.

debug Boolean. Generate debug output.

uw. summaryBoolean. Generate an uwerr summary plot.Generic graphical parameters to be passed on.

148 pointswithslantederror

Value

Returns a data.frame with named columns val, dval, tauint, dtauint, Wopt and stringsAsFactors, see uwerr.

```
pointswithslantederror
```

pointswithslantederror

Description

This function plots points with x- and y-errors visualised as a slanted errorbar. The length of the error bar represents x- and y-errors added in quadrature. The slope of the error bar is positive of negative depending on whether the correlation betwenn x and y is positive or negative, respectively.

Usage

```
pointswithslantederror(x, y, dx, dy, cor, col = "black", bcol = "black",
...)
```

Arguments

| X | numeric vector. x-values |
|------|--|
| У | numeric vector. y-values |
| dx | numeric vector. x-standard errors |
| dy | numeric vector. y-standard errors |
| cor | numeric vector. Correlation coefficients between x- and y- errors. |
| col | the color of the points |
| bcol | the color of the slanted error bars |
| | further graphical parameters to be passed on to points |

Details

plots data points with slanted error bars

Examples

```
x \leftarrow c(1:5)

y \leftarrow x^2

dx \leftarrow c(0.1, 0.2, 0.2, 0.1, 0.05)

dy \leftarrow c(0.05, 0.2, 0.1, 0.2, 0.1)

cor \leftarrow c(1, -1, -1, 1, 1)

plot(NA, xlim=range(x), ylim=range(y), xlab="y", ylab="y")

pointswithslantederror(x=x, y=y, dx=dx, dy=dy, cor=cor)
```

predict.bootstrapfit 149

Description

Predict values for bootstrapfit

Usage

```
## S3 method for class 'bootstrapfit'
predict(object, x, error = object$error.function, ...)
```

Arguments

object Object of type bootstrapfit.

x Numeric vector with independent variable.error Function to compute error from samples.

... additional parameters to be passed on to the prediction function.

Value

List with independent variable x, predicted central value val, error estimate err and sample matrix boot.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit(), print.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

Description

Print a bootstrap NLS fit

```
## S3 method for class 'bootstrapfit'
print(x, ..., digits = 2)
```

print.cf

Arguments

x object returned by bootstrap.nlsfit

... Additional parameters passed to the summary.bootstrapfit function.

digits number of significant digits to print in summary or print.

Value

No return value.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), simple.nlsfit(), summary.bootstrapfit()
```

print.cf

print.cf

Description

print.cf

Usage

```
## S3 method for class 'cf'
print(x, ...)
```

Arguments

x Object of type cf

... Generic parameters to pass on.

Value

No return value, only output is produced.

print.effectivemassfit 151

```
print.effect ive {\it mass fit}\\ print.effect ive {\it mass fit}
```

Description

print.effectivemassfit

Usage

```
## S3 method for class 'effectivemassfit'
print(x, ..., verbose = FALSE)
```

Arguments

x Object of class effectivemass... Additional parameters to be passed on.verbose Boolean. More verbose output.

Value

No return value.

print.ofit

print.ofit

Description

print.ofit

Usage

```
## S3 method for class 'ofit'
print(x, ...)
```

Arguments

x Object of type of it... Generic parameters to pass on.

Value

No return value.

152 pscor.sample

print.raw_cf

Print summary of data contained in raw_cf container

Description

Print summary of data contained in raw_cf container

Usage

```
## S3 method for class 'raw_cf'
print(x, ...)
```

Arguments

x raw_cf container with data and meta-data

... ignored

Value

See summary.raw_cf.

pscor.sample

 $Sample\ pseudoscalar\ correlator$

Description

Sample data for a pseudoscalar correlator for time extent Time=48.

Format

```
list of 2 elements: "t" "ps"
```

Examples

```
data("pscor.sample")
```

153 raw_cf

raw_cf

Container for raw correlation functions

Description

This function raw_cf() creates containers for raw correlation functions of class raw_cf. This class is particularly designed to deal with complex and matrix-valued correlation functions emerging in statistical mechanics and quantum field theory simulations. Arithmetic operations are defined for this class and utility functions such as is.raw_cf and is_empty.raw_cf.

Usage

```
raw_cf()
```

Value

An object of S3 class raw_cf.

See Also

Other raw_cf constructors: raw_cf_data(), raw_cf_meta()

raw_cf_data

Original data mixin constructor for raw_cf

Description

Original data mixin constructor for raw_cf

Usage

```
raw_cf_data(cf, data)
```

Arguments

cf

raw_cf object to extend.

data

Numeric or complex array, original data for all observables and measurements. This should have dimensions c(Nmeas,cf\$Timecf\$nrObscf\$nrStypes,cf\$dim). Having the internal dimensions innermost is not as efficient, but it allows different transformations to be applied to different observables in the same container

more easily.

Value

An object of S3 class raw_cf with original data mixin added.

raw_cf_meta

See Also

```
Other raw_cf constructors: raw_cf(), raw_cf_meta()
```

raw_cf_meta

raw_cf metadata mixin constructor

Description

raw_cf metadata mixin constructor

Usage

```
raw_cf_meta(cf = raw_cf(), nrObs = 1, Time = NA, nrStypes = 1,
  dim = c(1, 1), nts = Time)
```

Arguments

| cf | initial raw_cf object |
|----------|--|
| nr0bs | Integer, number of different observables assembled in the data field of this container. |
| Time | Integer, full time extent. |
| nrStypes | Integer, number of smearing types. |
| dim | Integer vector of "internal" dimensions for matrix-valued correlation functions. For a scalar correlation, this should be specified as c(1,1). |

Integer, number of time separations actually stored in the data field.

Value

nts

An object of S3 class raw_cf with metadat mixing added.

See Also

```
Other raw_cf constructors: raw_cf(), raw_cf_data()
```

raw_cf_to_cf

| raw_cf_to_cf | Extract a particular internal component of a 'raw_cf' into a 'cf' |
|---------------|---|
| 1 dw_c1_c0_c1 | Extract a particular internal component of a raw_cf into a cf |

Description

Extract a particular internal component of a 'raw_cf' into a 'cf'

Usage

```
raw_cf_to_cf(x, component)
```

Arguments

x 'raw_cf' container with 'raw_cf_data' and 'raw_cf_meta'

component Integer vector of the same length as the internal dimension of the 'raw_cf' spec-

ifying which component should be extracted.

Value

'cf' object

| readbinarycf read correlation function from binary files | |
|--|--|
|--|--|

Description

Reads a correlation function from binary files, including hdf5 formatted files.

Usage

```
readbinarycf(files, Time, obs = 5, Nop = 1, symmetrise = TRUE,
  endian = "little", op = "aver", excludelist = c(""), sym = TRUE,
  path = "", hdf5format = FALSE, hdf5name, hdf5index = c(1, 2))
```

Arguments

| files | list of filenames to be read. Can be created using getorderedfilelist. The filelist is assumed to be order according to ascending gauge fields. |
|-------|---|
| Time | time extent of correlation functions. |
| obs | each file may contain many correlation functions. With 'obs' one choses which observable to read in. To be precise, in each file the reading will start at point Timeobssizeof(complex <double>) and read NopTimesizeof(complex<double>).</double></double> |
| Nop | number of replicas for the correlator to read in. |

symmetrise symmetrise the correlation function or not

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endian the endianess of the binary file.

op the N replicas can be either averaged (op="aver") or summed (op="sum").

excludelist files to exclude from reading.

sym if TRUE average C(+t) and C(-t), otherwise C(+t) and -C(-t).

path path to be prepended to every filename. hdf5format if TRUE, try to read from an hdf5 file.

hdf5name Name of the data set as a string.

hdf5index The data might be an array of size n x Time. hdf5index is used to convert two

columns of the data to a complex valued vector using the first and second index for real and imaginary part, respectively. If hdf5index has length smaller than

2 the first index is reused.

Details

It is assumend that each file contains at least (obs+N)*Time complex doubles, where Time is the time extent, obs is the number of the observable to read in and Nop the number of replicas for this observable. It is assumed that complex is the fastest running index, next time and then obs. The filelist is assumed to be ordered according to the gauge configuration MC history.

Value

returns a list with two arrays cf and icf with real and imaginary parts of the correlator, and integers Time, nrStypes=1 and nrObs=1. Both of the arrays have dimension c(N, (Time/2+1)), where N is the number of measurements (gauges). Time is the time extent, nrStypes the number of smearing levels and nrObs the number of operators, both of which are currently fixed to 1.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

readcmidatafiles, readbinarydisc, readcmidisc, readcmicor

Examples

readbinarydisc 157

| readbinarydisc | read disconnected loops from binary files | |
|----------------|---|--|
|----------------|---|--|

Description

Reads disconnected loops from binary files.

Usage

```
readbinarydisc(files, Time = 48, obs = 5, endian = "little",
  excludelist = c(""), nrSamples = 1, path = "")
```

Arguments

files list of filenames to be read. Can be created for instance using getorderedfilelist.

The filelist is assumed to be ordered with number of samples running fastest, and

the next to fastest nubmer of gauges.

Time time extent of correlation functions.

obs each file may contain Time*obs correlation functions. With obs one choses

which observable to read in.

excludelist the endianess of the binary file. excludelist files to exclude from reading.

nrSamples the number of samples

path path to be prepended to every filename.

Details

It is assumend that each file contains O*Time complex doubles, where Time is the time extent and O the number of observables in the file. It is assumed that complex is the fastest running index, next time and then observables. The different samples are assumend to be in different files. The file list is assumed to be ordered with number of samples running fastest, and then number of gauges.

Value

returns a list with two arrays cf and icf with real and imaginary parts of the loops, and integers Time, nrStypes=1, nrSamples and nrObs=1. Both of the arrays have dimension c(Time, N), where N is the number of measurements (gauges) and Time the time extent, nrStypes the number of smearing levels and nrObs the number of operators, both of which are currently fixed to 1.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

readcmidatafiles, readbinarycf, readcmidisc, readcmicor

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Examples

```
## running toy example
file <- paste0(system.file("extdata", package = "hadron"), "/C2_pi0.dat")
X <- readbinarydisc(files=file, Time=64, obs=0)
X$cf

## more realistic example
## Not run: files <- character()
## Not run: for(i in seq(600,1744,8))
## Not run: files <- c(files, "C2_dis_u_conf", sprintf("%.04d", i), ".dat", sep="")
## Not run: cf <- readbinarydisc(files, obs=4, excludelist=c("C2_pi0_conf0632.dat"))</pre>
```

readbinarysamples

Read binary correlation function by sample

Description

Read binary correlation functions sample by sample, return as a list of length nosamples where increasing indices refer to averaging over increasing numbers of samples.

Usage

```
readbinarysamples(files, Time = 48, nosamples = 2, endian = "little",
  excludelist = c(""), sym = TRUE, path = "", ftype = double())
```

Arguments

files character vector. Paths to the file to read. As path is prepended to each element,

one can also just pass the filenames here.

Time numeric. Time extent. nosamples number of samples

endian character, either little or big.

excludelist character vector. Elements in files that are specified in excludelist are

skipped. The caller could also just pass setdiff(files, excludelist).

sym logical. Whether the read data shall be symmetrized in the end.

path character. Path that is prefixed to each of the paths given in files.

ftype numeric type. As the data is read in binary this type has to match exactly the

one in the file.

Value

Returns a list of cf objects.

readcmidisc 159

| readcmidisc reads disconnected loops in cmi format |
|--|
|--|

Description

reads disconnected loops in cmi (Chris Michael) format from a list of files.

Usage

```
readcmidisc(files, obs = 9, ind.vec = c(2, 3, 4, 5, 6, 7, 8),
  excludelist = c(""), skip = 0, L, colClasses = c("integer", "integer", "integer", "numeric", "numeric", "numeric", "numeric", "numeric"),
  debug = FALSE)
```

Arguments

files list of filenames to be read. Can be created using getorderedfilelist.

obs index of operator to parse from files

ind. vec vector containing the index (column in file) of obs, t, samples, Re(local), Im(local,

Re(smeared), Im(smeared).

excludelist files to exclude from reading.

skip lines to skip at beginning of each file.

the spatial lattice extent, set to Time/2 if missing. colClasses

The column data type classes, the read.table.

debug setting debug to TRUE makes the routine more verbose by spilling out separate

filenames.

Value

returns a list with four arrays cf, icf scf and sicf containing real and imaginary parts of the local and smeared loops, respectively, and integers Time, nrStypes=2, nrSamples and nrObs=1. The four arrays have dimension c(Time, S, N), where S is the nubmer of samples, Time is the time extent and N is the number of measurements (gauges). Time is the time extent, nrStypes the number of smearing levels and nrObs the number of operators, which are currently fixed to 1 and 2, respectively. nrSamples is the number of samples.

Note that the arrays are normalised by $1/sqrt(L^2)$.

The routine expects that all files have identical content. Otherwise the routine will stop.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

readcmidatafiles, readbinarycf, readbinarydisc, readcmicor

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Examples

```
# a running toy example
hpath <- system.file(package="hadron")
files <- paste0(hpath, "/extdata/newdisc.0.1373.0.006.k0v4.10")
X <- readcmidisc(files=files)
X

## a more realistic example
## Not run: v4files <- character()
## Not run: for(i in seq(600,1744,8))
## Not run: v4files <-
## Not run: v4files <-
## Not run: v4files <-
## Not run: v4files, paste("disc.0.163265.0.006.k0v4.", sprintf("%.04d", i), sep=""))
## Not run: v4data <- readcmidisc(v4files)</pre>
```

readcmifiles

Read Single Data Files in Chris Michael Format

Description

reads data from single files in Chris Michael format

Usage

```
readcmifiles(files, excludelist = c(""), skip, verbose = FALSE, colClasses,
  obs = NULL, obs.index, avg = 1, stride = 1)
```

Arguments

files list of filenames to be read. Can be created using getorderedfilelist.

excludelist files to exclude from reading.

skip Number of lines to be skipped at the beginning of each file

verbose Increases verbosity of the function.

colClasses The column data type classes, the read. table.

obs To reduce memory consumption it is possible to extract only one of the obser-

vales. The column in which to match obs is to be given with obs.index. This

will only be affective if obs is not NULL.

obs.index The column in which to match obs is to be given with obs.index.

avg Integer. Average over successive number samples

stride Integer. Read only subset of files with corresponding stride.

readcmifiles 161

Details

These functions reads data from single data files. It is assumed that every file has the same number of columns.

The cmi (Chris Michael) format for connected correlators comprises 6 colums per file: 1) the observable type number (itype); 2) the operator type number (iobs); 3) the time difference from source going from 0 to Time/2 for each operator type; 4) c_1 correlator value at time value forward in time; 5) c_2 correlator value at time value backward in time; 6) number of gauge configuration.

There are scripts shipped with the package converting the output written into seperate files for each gauge configuration into the expected format. They are called puttogether.sh and puttogether_reverse.sh which will sort with increasing and with decreasing gauge configuration number, respectively.

Note, that the normalisation of correlators needs multiplication by factor of 0.5 (and possible $(2*\kappa)^2$ and L^3 factors dependent on your conventions).

The values of itype run from 1 to the total number of gamma matrix combinations available. iobs equals 1 for local-local correlators, 3 for local-smeared, 5 for smeared-local and 7 for smeared-smeared

```
For charged mesons the order of gamma-matrix combinations is as follows: order PP PA AP AA 44 P4 4P A4 4A for pion like P=\gamma_5 A=\gamma_4\gamma_5 4=\gamma_4 order 44 VV AA 4V V4 4A A4 VA AV for rho-a1 like 4=\gamma_i\gamma_4 V=\gamma_i A=\gamma_i\gamma_5 order BB SS - total 20 \gamma_i\gamma_4\gamma_5 S=I itype=21 is conserved vector current at sink, \gamma_5 at source
```

For neutral mesons the order of gamma-matrix combinations is as follows: order PP PA AP AA II PI IP AI IA for pion like $P=\gamma_5$ $A=\gamma_4\gamma_5$ I=1 order 44 VV BB 4V V4 4B B4 VB BV for rho-b1 like $4=\gamma_i\gamma_4$ $V=\gamma_i$ $B=\gamma_i\gamma_4\gamma_5$ order XX AA - total 20 for a0-X like $A=\gamma_i\gamma_5$ $X=\gamma_4$

For loops (disconnected contributions to neutral mesons) the convention is as follows: files are assumed to have eight columns with gauge, gamma, t, sample, ReTL, ImTL, ReTF, ImTF, where gamma is 1 to 16 as list of (hermitian) gamma matrices: order g_5 g_1 g_2 g_3

```
-ig_4* g_5 g_1 g_2 g_3

-ig_5* ig_5 g_1 g_2 g_3 ie 1,...

-ig_5g_4 -ig_5 g_1 g_2 g_3 ie g_4, g_5row 2

(so P is 1; A4 is 5; S is 9; A_i is 10,11,12 etc)
```

t is t-value of trace (here spatial momentum is zero) sample is sample number 1,...24 (or 96) ReTL is real part of trace at time t, with gamma combination given and Local operator (F is Fuzzed == non-local) operator).

Normalisation is trace M^-1 with M=1+...

To make a disconnected correlator, one combines these traces for different t (and different sample number) as a product. Note only Re Gamma=1 and Im Gamma=gamma_5 have VEV's, see computeDisc

Value

readcmicor returns an object of class cmicor, read from a single file.

readcmidatafiles returns an object of class cmicor, which is an rbind of all data. frames read from the single files in the filelist.

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readcmiloopfiles returns an object of class cmiloop, which is an rbind of all data. frames read from the single files in the filelist.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

```
getorderedfilelist, extract.obs, readcmidisc
```

Examples

readgradflow

Read Gradient Flow Output Files in tmLQCD format

Description

given a pathname, reads all gradient flow output files in that directory

Usage

```
readgradflow(path, skip = 0, basename = "gradflow", col.names)
```

Arguments

path the path into which the function should descend

skip number of measurements to skip. basename basename of the files to be read.

col.names column names of the columns in the files to be read. If not given it will be

infered from the files, if possible.

Details

This function reads all tmLQCD gradient flow files in the given path and returns a data frame which concatenates them all.

The single files are expected to be in the tmLQCD format which consists of a header with the column names "traj t P Eplaq Esym tsqEplaq tsqEsym Wsym" and the measurement for each flow time in rows. The columns can be ordered arbitrarily as long as the header and the data are consistent.

readhlcor 163

Value

The function returns a data frame ordered first by the flow time and then by the trajectory number (so the trajectory number is the index which runs fastest). The data frame has column names

- t flow time
- traj trajectory number
- P plaquette expectation value (at flow time t)
- Eplaq energy density from plaquette definition (at flow time t)
- Esym energy density from clover definition (at flow time t)
- tsqEplaq flow time squared multiplied by plaquette energy density
- tsqEsym flow time squared multiplied by clover energy density
- Wsym BMW 'w(t)' observable

.

Author(s)

Bartosz Kostrzewa, <bartosz.kostrzewa@desy.de>

Examples

```
path <- system.file("extdata/", package="hadron")
raw.gf <- readgradflow(path)</pre>
```

readhlcor

readhlcor

Description

readhlcor

Usage

```
readhlcor(filename)
```

Arguments

filename

String. Filename of the heavy light correlator data file. The file is expected to have nine columns, the first four integer, the second four numeric and the last integer valued again.

Value

Invisibly returns a data.frame object containing the file content.

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readnissatextcf

reader for Nissa text format correlation functions

Description

reader for Nissa text format correlation functions

Usage

```
readnissatextcf(file_basenames_to_read, smear_combs_to_read, Time,
  combs_to_read, nts = Time, sym.vec = c(1), symmetrise = FALSE)
```

Arguments

file_basenames_to_read

Character vector of file names without the smearing combination suffixes (such as 'll', 'ls', 'sl', 'ss') which will be added in the reading routine accordign to what was passed via smear_combs_to_read. An example would be '0001/mes_contr_2pts', not the lack of the smearing suffix.

smear_combs_to_read

Character vector containing the smearing cominations that are to be read. These will be attached to the file_basenames_to_read in the reading routine.

Time Integer, time extent of the lattice.

combs_to_read Data frame co

Data frame containing the indices of the masses and r-paramter combinations to be read as well as the name of the spin combination. For a two-point function using the second and third mass (0-indexed), the (+^dag,+) r-combination and the pseudoscalar-pseudoscalar spin combination would look as follows:

nts Integer, number of time slices to be read from the correlator files.

sym.vec Integer or numeric vector. Specifies whether the correlator at the given posi-

tion is symmetric (+1.0) or anti-symmetric (-1.0) under time reflection. This is passed to symmetrise.cf. This should be of sufficient length to cover all correlators that are going to be read (one number per row of combs_to_read and per

entry of smear_combs_to_read)

symmetrise Boolean, specifies whether averaging over backward and forward correlators

should be done after the correlator has been read in.

Value

Returns an object of class cf.

readoutputdata 165

readoutputdata

Read Data In output.data Format of tmLQCD

Description

reads data from an output.data file written by tmLQCD

Usage

```
readoutputdata(filename)
```

Arguments

filename

filename of the data file

Details

The data can be plotted directly using "plot".

Value

returns a data frame of class "outputdata" containing the data.

Returns an object of class outputdata derived from a data.frame as generated by read.table applied to the input file.

Author(s)

Carsten Urbach < curbach@gmx.de>

Examples

```
plaq <- readoutputdata(paste0(system.file(package="hadron"), "/extdata/output.data"))
plot(plaq)</pre>
```

readtextcf

Read correlator data from single file

Description

Reads arbitrary number of samples for a complex correlation function from a text file.

```
readtextcf(file, Time = 48, sym = TRUE, path = "", skip = 1,
  check.t = 0, ind.vector = c(2, 3), symmetrise = TRUE, stride = 1,
  avg = 1, Nmin = 4, autotruncate = TRUE)
```

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Arguments

file filename of file to read from.

Time time extent of the correlation function

sym if TRUE average C(+t) and C(-t), otherwise C(+t) and -C(-t). Averaging can be

switched off using the symmetrise option.

path the path to the files.

skip number of lines to skip at beginning of file

check.t if set to an integer value larger than zero the function will assume that in the

corresponding column of the file the Euclidean time is counted and it will check

whether the maximum in this column is identical to Time-1.

ind. vector index vector of length 2 with the indices of real and imaginary values of corre-

lator, respectivley.

symmetrise if set to TRUE, the correlation function will be averaged for t and Time-t, with

the sign depending on the value of sym. Note that currently the correlator with

t-values larger than Time/2 will be discarded.

stride Integer. Read only subset of files with corresponding stride.

avg Integer. Average over successive number samples

Nmin Integer. Minimal number of measurements that must remain after sparsification

and averaging. Default equals to 4.

autotruncate Boolean. Whether to autotruncate or not

Value

returns a list with two arrays cf and icf with real and imaginary parts of the correlator, and integers Time, nrStypes=1 and nrObs=1. Both of the arrays have dimension c(N, (Time/2+1)), where N is the number of measurements (gauges). Time is the time extent, nrStypes the number of smearing levels and nrObs the number of operators, both of which are currently fixed to 1.

Author(s)

Carsten Urbach, <curbach@gmx.de>

See Also

readcmidatafiles, readbinarydisc, readcmidisc, readcmicor, readbinarycf

removeTemporal.cf 167

removeTemporal.cf

Remove Thermal States by Weighting and Shifting

Description

Remove Thermal States by Weighting and Shifting

Usage

```
removeTemporal.cf(cf, single.cf1, single.cf2, p1 = c(0, 0, 0), p2 = c(0, 0, 0), L, lat.disp = TRUE, weight.cosh = FALSE)
```

Arguments

| cf | Object of type cf |
|-------------|---|
| single.cf1 | Object of type cf |
| single.cf2 | Object of type cf |
| p1 | Numeric vector. Spatial momentum of first state |
| p2 | Numeric vector. Spatial momentum of second state |
| L | Integer. Spatial lattice extent. |
| lat.disp | Boolean. Use lattice dispersion relation instead of continuum one |
| weight.cosh | Boolean. Use cosh functional form in the weighting procedure |

Value

weighted and shifted correlation function as a cf object.

resample_hankel

Resample bootstrap samples in Hankel effmass

Description

The bootstrap distribution in the Hankel effective mass can be quite broad due to outliers and long tails. These screw with proper error estimation. Therefore it can be useful to trim these tails. Just trimming a bootstrap distribution would lead to less samples, therefore we do a parametric resampling.

Usage

```
resample_hankel(hankel_effmass, distance = 5)
```

Arguments

```
hankel_effmass Hankel effective mass from hankel2effmass.
distance Numeric, threshold for marking outliers.
```

Details

The central values are also inferred from the distribution because they often are outliers themselves. The new central value is the middle between the upper and lower quantile, making the resulting distribution symmetric.

Half the distance between the quantiles is taken to be the error, therefore the quantiles are chosen at 16 and 84 percent to match the standard deviation. All points that are more than "distance" errors away from the new central value are taken to be outliers.

Value

The Hankel effmass object is returned with the same fields, the numbers have been changed. Additionally there are the followi1ng fields:

- cov_full contains the full covariance matrix as determined from all the data. This will be skewed by the outliers.
- finite_count gives the number of non-outliers per time slice.
- complete_count gives the numbers of complete cases if all outliers are taken out. This number is often zero because the late time slices contain lots of outliers due to the noise.
- cov_3sigma_pairwise is the covariance matrix using only the non-outliers and removing NAs in a pairwise fashion, using the maximum of the data. This is the covariance matrix that is used for the resampling.

In case that no time slices had a finite error estimate, this function returns just NA.

```
resampling_is_compatible
```

Checks whether the resampling of two cf objects is compatible

Description

Checks whether the resampling of two cf objects is compatible

Usage

```
resampling_is_compatible(cf1, cf2)
```

Arguments

```
cf1 cf object with cf_boot
cf2 cf object with cf_boot
```

Details

Checks whether operations such as addition can be performed on the resampling samples of cf1 and cf2. In addition to all meta parameters, the dimensions of the resampling sample arrays must be identical.

Value

List of named booleans for each of the checked conditions with elements boot, boot.R, boot.l, sim, endcorr, resampling_method, boot_dim, icf and, optionally iboot_dim (if both cf1 and cf2 contain imaginary parts).

```
resampling_is_concatenable
```

Checks whether the resampling of two cf objects is concatenable

Description

Checks whether the resampling of two cf objects is concatenable

Usage

```
resampling_is_concatenable(cf1, cf2)
```

Arguments

```
cf1 cf object with cf_boot
cf2 cf object with cf_boot
```

Details

In contrast to resampling_is_compatible, this function checks if the resampling samples are concatenable on the horizontal axis. In addition to checking all meta parameters, the number of rows in the resampling arrays must be identical but the number of columns may differ.

Value

List of named booleans for each of the checked conditions with elements boot, boot.R, boot.l, sim, endcorr, resampling_method, boot_nrow, icf and, optionally iboot_nrow (if both cf1 and cf2 contain imaginary parts).

residual_plot

residual_plot

Description

```
generic residual_plot method
```

```
residual_plot(x, ...)
```

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Arguments

x the object to plot

... additional parameters to be passed on to specialised functions

Value

No return value.

restore_seed

Restore random number generator state

Description

Restore random number generator state

Usage

restore_seed(old_seed)

Arguments

old_seed

integer. Previous seed that should be restored globally.

Value

No return value, but the random seed is reset to old_seed.

samplecf

Sample cf data

Description

Sample data for a correlation function for a 24 cube times 48 lattice QCD simulation representing a pion propagation. It is stored in form of an object of class cf, which is derived from list.

Format

The format is: List of 15 \$ cf : num 521 533 532 531 561 ... \$ icf : num 521 533 532 531 561 ... \$ Time : num 48 \$ nrStypes : num 1 \$ nrObs : num 1 \$ boot.samples : logi TRUE \$ jackknife.samples: logi FALSE \$ symmetrised : logi TRUE \$ boot.R : num 1500 \$ boot.l : num 2 \$ seed : num 1442556 \$ sim : chr "geom" \$ cf0 : num 519 375 274 221 185 ... \$ cf.tsboot :List of 11 ...\$ t0 : num 519 375 274 221 185\$ t : num 521 518 520 519 519\$ R : num 1500 ...\$ data : num 521 533 532 531 561\$ seed : int 403 624 -867935848 1692432057 -1535150298 -1438296209 912697060 1838233749 1438572626 999279531\$ statistic:function (x) ...\$ sim : chr "geom" ...\$ n.sim : int 1018 ...\$ call : language tsboot(tseries = cf\$cf, statistic = function(x) return(apply(x, MARGIN = 2L, FUN = mean)) ...) ...\$ 1 : num 2 ...\$ endcorr : logi TRUE ... attr(, "class") = chr "boot" ... - attr(, "boot_type") = chr "tsboot" \$ tsboot.se : num 1.001 0.615 0.572 0.537 0.499 ... - attr(*, "class") = chr "cf" "list"

shift.cf 171

Examples

```
data(samplecf)
bootstrapped <- bootstrap.cf(samplecf)
plot(bootstrapped)</pre>
```

shift.cf

shift a correlation function by 'places' time-slices

Description

C'(t) = C(t+places) where places can be positive or negative as required and periodic boundary conditions in time are assumed

Usage

```
shift.cf(cf, places)
```

Arguments

cf unsymmetrised correlation function (cf_meta and cf_orig mixins required)

places integer number of time-slices for backward (negative) or forward (positive) shifts

Value

Returns an object of class cf containing the shifted correlation function.

shift.raw_cf

shift a raw_cf correlation function by 'places' time-slices

Description

shift a raw_cf correlation function by 'places' time-slices

```
shift.raw_cf(cf, places)
```

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Arguments

cf

raw_cf container

places

Integer (possibly a vector), number of time slices that the correlation function should be shifted by. Can be positive or negative. This can either be a single value such that a shift by this many time slices will be applied to every measurement or it can be a vector of values of the same length as the number of measurements in cf. In that case, a different shift will be applied to each measurement. This is useful if it is important to preserve the absolute time coordinates of a correlation function until some time-dependent transformations have been applied.

Details

The correlation funtion C(t) is shifted in time to produce:

$$C'(t) = C(t + places)$$

using periodic boundary conditions in time.

Value

Returns an object of class raw_cf, shifted compared to the input object.

simple.nlsfit

NLS fit with without bootstrap

Description

NLS fit with without bootstrap

Usage

```
simple.nlsfit(fn, par.guess, y, x, errormodel, priors = list(param = c(), p =
c(), psamples = c()), ..., lower = rep(x = -Inf, times =
length(par.guess)), upper = rep(x = +Inf, times = length(par.guess)), dy,
dx, CovMatrix, boot.R = 0, gr, dfn, mask, use.minpack.lm = TRUE,
error = sd, maxiter = 500, success.infos = 1:3,
relative.weights = FALSE, na.rm = FALSE)
```

Arguments

fn

fn(par, x, ...). The (non-linear) function to be fitted to the data. Its first argument must be the fit parameters named par. The second must be x, the explaining variable. Additional parameters might be passed to the function. Currently we pass boot.r which is 0 for the original data and the ID (1, ...) of the bootstrap sample otherwise. As more parameters might be added in the future it is recommended that the fit function accepts ... as the last parameter to be forward compatible.

simple.nlsfit 173

par.guess initial guess values for the fit parameters.

the data as a one-dimensional numerical vector to be described by the fit func-

tion.

x values of the explaining variable in form of a one-dimensional numerical vector.

errormodel Either "yerrors" or "xyerrors", depending on the x-values having errors or not.

priors List possessing the elements param, p and psamples. The vector param in-

cludes the indices of all fit parameters that are to be constrained and the vector p the corresponding paramater values (e.g. known from a previous fit). The list element psamples is a matrix of dimensions (boot.R, length(param)) and contains the corresponding bootstrap samples. If this list is not specified priors

are omitted within the fit.

... Additional parameters passed to fn, gr and dfn.

lower Numeric vector of length length(par.guess) of lower bounds on the fit pa-

rameters. If missing, -Inf will be set for all.

upper Numeric vector of length length(par.guess) of upper bounds on the fit pa-

rameters. If missing, +Inf will be set for all.

dy, dx Numeric vector. Errors of the dependent and independent variable, respectively.

These do not need to be specified as they can be computed from the bootstrap samples. In the case of parametric bootstrap it might would lead to a loss of information if they were computed from the pseudo-bootstrap samples. They

must not be specified if a covariance matrix is given.

CovMatrix complete variance-covariance matrix of dimensions c(length(y), length(y))

or c(length(y)+length(x),length(y)+length(x)) depending on the errormodel. Pass NULL if the matrix has to be calculated from the bsamples. In that case, if the number of boostrap samples is small compared to the number of variables, singular value decomposition with small eigenvalue replacement will be used (see invertCovMatrix) to attempt a clean inversion. In case a variance-covariance matrix is passed, the inversion will simply be attempted using solve on the Cholesky decomposition. Finally, if CovMatrix is missing, an uncorre-

lated fit will be performed.

boot.R If larger than 0, boot.R parameteric bootstrap samples are generated on the fit

results after fit and error calculation are finished. The original data is never

boostraped in this function.

gr gr(par, x, ...). gr=d(fn) / d(par) is a function to return the gradient of fn.

It must return an array with length(x) rows and length(par) columns.

dfn dfn(par, x, ...). dfn=d(fn) / dx is the canonical derivative of fn by x and

only relevant if x-errors are provided.

mask logical or integer index vector. The mask is applied to select the observations

from the data that are to be used in the fit. It is applied to x, y, dx, dy, bsamples

and CovMatrix as applicable.

use.minpack.lm use the minpack.lm library if available. This is usually faster than the default

optim but somtimes also less stable.

error Function that takes a sample vector and returns the error estimate. This is a

parameter in order to support different resampling methods like jackknife.

174 store_correl

maxiter integer. Maximum number of iterations that can be used in the optimization

process.

integer vector. When using minpack.1m there is the info in the return value. Values of 1, 2 or 3 are certain success. A value of 4 could either be a success or a saddle point. If you want to interpret this as a success as well just pass 1:4 instead of the default 1:3.

relative.weights

success.infos

are the errors on y (and x) to be interpreted as relative weights instead of absolute ones? If TRUE, the covariance martix of the fit parameter results is multiplied by $\frac{2}{dof}$. This is the default in many fit programs, e.g. gnuplot.

na.rm logical. If set to true, NAs in y and dy will be ignored. If x-errors are taken

into account, NAs in x and dx will be ignored, too.

Value

Returns an object of class bootstrapfit, see bootstrap.nlsfit.

See Also

Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), summary.bootstrapfit()

Examples

```
## Declare some data.
value <- c(0.1, 0.2, 0.3)
dvalue <- c(0.01, 0.01, 0.015)
x <- c(1, 2, 3)
dx <- c(0.1, 0.1, 0.1)

fn <- function (par, x, ...) par[1] + par[2] * x

fit.result <- simple.nlsfit(fn, c(1, 1), value, x, "xyerrors", dy=dvalue, dx=dx)
summary(fit.result)</pre>
```

store_correl

Store a 'raw_cf' correlator in an associative array together with a description The object cf will be stored as an element of cmap under key out_key in the member obj of cmap. The data frame passed via desc will be appended as a row to cmap[[out_key]]\$map. If out_key does not exist as a key in cmap, a new element will be created. If it already exists, addStat.raw_cf is called to add statistics to the existing raw_cf. Requires the 'hash' package.

string2error 175

Description

Store a 'raw_cf' correlator in an associative array together with a description The object cf will be stored as an element of cmap under key out_key in the member obj of cmap. The data frame passed via desc will be appended as a row to cmap[[out_key]]\$map. If out_key does not exist as a key in cmap, a new element will be created. If it already exists, addStat.raw_cf is called to add statistics to the existing raw_cf. Requires the 'hash' package.

Usage

```
store_correl(cmap, cf, out_key, desc)
```

Arguments

cmap Object of class hash to act as storage for 'raw_cf' correlators.

cf Object of class raw_cf to be stored in cmap.

out_key String, key associated with cf object to be stored in cmap.

desc Single row data frame containing some descriptive parameters for cf.

Value

Since objects of class hash are passed and modified by reference, there is no explicit return value. Instead, the passed cmap is modified.

string2error string2error

Description

takes a string of the form "x(dx)", where dx are the error digits and returns a numeric vector c(x, y), where y is dx as a proper numeric value.

Usage

```
string2error(x)
```

Arguments

x Input character string.

Details

can be used in combination with apply

Value

a numeric vector with the first element the value and the second the error

176 subtract.excitedstates

Examples

```
string2error("0.35667(25)")
s <- c("0.35667(25)", "0.667(50)")
apply(array(s, dim=c(1, length(s))), 2, string2error)</pre>
```

subtract.excitedstates

Substract excited states.

Description

Excited states are subtracted from the given correlation function and matching matrixfit. The fit is usually done on late time slices when the thermal states have decayed so much that they can be neglected. On the early time slices there are contributions which cannot be explained with a single cosh (or sinh) function. These are exactly the contributions that we do not want.

Usage

```
subtract.excitedstates(cf, mfit, from.samples = FALSE)
```

Arguments

cf Correlation function of class cf.

mfit Fit result of class matrixfit.

from. samples Whether to use existing bootstrap samples. If set to TRUE, the same operation

will be applied to the bootstrap samples. Otherwise the result will not contain

bootstrap samples, even if the input correlation function did.

Details

The correlation function is altered on the time slices which are earlier than the start of the fit interval. The correlator is replaced by the model function (cosh or sinh or exp) extrapolated until the first time slice. The deviations of the (bootstrap) samples from the mean value are kept.

Value

A correlation function of class cf which is computed from the old correlation function C(t) as $M(t)+C(t)-\bar{C}(t)$, where M(t) is the fit model and $\bar{C}(t)$ denotes the average over the (bootstrap) samples. Only time slices earlier than the fit are altered.

summary.bootstrapfit 177

```
summary.bootstrapfit Summarize a bootstrap NLS fit
```

Description

Summarize a bootstrap NLS fit

Usage

```
## S3 method for class 'bootstrapfit'
summary(object, ..., digits = 2,
    print.correlation = TRUE)
```

Arguments

```
object object returned by bootstrap.nlsfit
... ignored
digits number of significant digits to print in summary or print.
print.correlation
Logical. Whether to show the correlation between of the fit parameters.
```

Value

No return value.

See Also

```
Other NLS fit functions: bootstrap.nlsfit(), parametric.bootstrap(), parametric.bootstrap.cov(), parametric.nlsfit(), parametric.nlsfit.cov(), plot.bootstrapfit(), predict.bootstrapfit(), print.bootstrapfit(), simple.nlsfit()
```

```
summary.cf summary.cf
```

Description

```
summary.cf
```

```
## S3 method for class 'cf'
summary(object, ...)
```

178 summary.effectivemass

Arguments

object Object of type cf

... Generic parameters to pass on.

Value

No return value, only output is produced.

summary.coshfit

Summarize a cosh-fit

Description

Summarize a cosh-fit

Usage

```
## S3 method for class 'coshfit'
summary(object, verbose = FALSE, ...)
```

Arguments

object An object generated by fit.cosh.

verbose If set to TRUE, all fit results including the correlation matrix of the fit parameters

are showed. Otherwise only the effective mass with error is given.

... additional parameters to match generic summary arguments

Value

No return value.

```
summary.effectivemass summary.effectivemass
```

Description

summary.effectivemass

```
## S3 method for class 'effectivemass'
summary(object, ...)
```

Arguments

object Object of type effectivemass generated by fit.effectivemass

... Generic parameters to pass on.

Value

No return value.

```
\verb"summary.effective" mass fit
```

summary.effectivemassfit

Description

summary.effectivemassfit

Usage

```
## S3 method for class 'effectivemassfit'
summary(object, ..., verbose = FALSE)
```

Arguments

object Object of type cf

... Generic parameters to pass on.

verbose More verbose output.

Value

No return value.

```
\verb|summary.gevp.amplitude|\\
```

summary.gevp.amplitude

Description

```
summary.gevp.amplitude
```

```
## S3 method for class 'gevp.amplitude'
summary(object, ...)
```

Arguments

```
object Object of type gevp.amplitude.... Generic Parameters to be passed on.
```

Value

No return values.

summary.hadronacf

summary. hadron acf

Description

generic function to summarise an object of class "myGamma"

Usage

```
## S3 method for class 'hadronacf'
summary(object, ...)
```

Arguments

object Object of type hadronacf generated by computeacf

... Generic parameters to be passed on

Value

No return value.

```
\verb|summary.hankel_summed| summary.hankel_summed|
```

Description

```
summary.hankel_summed
```

Usage

```
## S3 method for class 'hankel_summed'
summary(object, ...)
```

Arguments

object Object of type "hankel_summed" generated by bootstrap.hankel_summed

... Generic parameters to pass on.

summary.matrixfit 181

Value

Returns invisibly a data frame with columns E, dE (energies and their standard errors) q16 and q84 the 16 and 84 percent quantiles.

summary.matrixfit

summary.matrixfit

Description

```
summary.matrixfit
```

Usage

```
## S3 method for class 'matrixfit'
summary(object, ...)
```

Arguments

object

Object of type matrixfit

. . .

Generic parameters to pass on.

Value

No return value.

summary.ofit

summary.ofit

Description

summary.ofit

Usage

```
## S3 method for class 'ofit'
summary(object, ...)
```

Arguments

object

Object of type of it

. . .

Generic parameters to pass on.

Value

No return value.

182 summary.uwerr

summary.raw_cf

Print summary of data contained in raw_cf container

Description

Print summary of data contained in raw_cf container

Usage

```
## S3 method for class 'raw_cf'
summary(object, ..., statistics = FALSE)
```

Arguments

object raw_cf container with data and meta-data

... ignored

statistics Boolean, return central value and error for all components of the 'raw_cf'. This

can be slow so the default is FALSE.

Value

The summary is returned invisibly in form of a data frame.

summary.uwerr

summary.uwerr

Description

summary.uwerr

Usage

```
## S3 method for class 'uwerr'
summary(object, ...)
```

Arguments

object Object of type uwerr

... Generic parameters to pass on.

Value

No return value.

swap_seed 183

| swap_seed | Set seed and store a seed which can be used to reset the random num- |
|-----------|--|
| | ber generator |
| | |

Description

Set seed and store a seed which can be used to reset the random number generator

Usage

```
swap_seed(new_seed)
```

Arguments

new_seed

integer. The new seed that is to be set. In case this is parameter is missing, no changes are made and the function just returns NULL. This is useful because a function can just pass on its own seed argument and therefore control whether the seed shall be fixed or left as-is.

Value

The generated seed is returned if it exists. Otherwise NULL. In case that new_seed was missing, NULL is returned.

symmetrise.cf

Average backward and forward-dominated parts of the correlation function

Description

When a correlation function is symmetric or anti-symmetric in time, this symmetry can be exploited by averaging the part from source-sink separation 1 to cf\$Time/2 with the part from cf\$Time/2+1 to cf\$Time-1 in order to improve statistical precision. This function reduces the number of time slices in a cf object from cf\$Time to cf\$Time/2+1 by performing this averaging.

Usage

```
symmetrise.cf(cf, sym.vec = c(1))
```

Arguments

cf Object of type cf.

sym.vec Integer or integer vector of length cf\$nrObs giving the time-reflection symmetry

(1 for symmetric, -1 for anti-symmetric) of the observable in question.

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Value

Returns an object of class cf, which is the symmetrised version of the input cf object.

takeTimeDiff.cf

Take time difference

Description

Performs the calculation of the shifted correlator $C_{\text{shift}}(t) = C(t) - C(t + / - \text{deltat})$.

Usage

```
takeTimeDiff.cf(cf, deltat = 1, forwardshift = FALSE)
```

Arguments

cf Object of type cf, a particle correlation function which shall be shifted.

deltat integer. the time shift

forwardshift boolean. If set to TRUE, the forward finite difference is used instead of the back-

ward one

Value

The shifted correlator as an object of type cf, see cf

tex.catwitherror

paste a number with error in tex-ready format

Description

A number with error is converted to a string in tex-ready format like xx(yy) thereby automatically determining the digit at which the error applies.

Usage

```
tex.catwitherror(x, dx, digits = 1, with.dollar = TRUE, with.cdot = TRUE,
...)
```

tikz.finalize 185

Arguments

| Х | either a single numeric value, or a numeric vector, where the first element is the value and the second is its error |
|-------------|---|
| dx | the error. If supplied, it will be printed as the error and the value is the first element of x. If dx is missing, the second element of x, if available, is used as the error. If dx is missing and the length of x is one, only the value is converted to a string without error. |
| digits | number of error digits |
| with.dollar | include the tex dollar in the return string or not |
| with.cdot | replace the "e" in scientific notation by tex-style "cdot" or not |
| | arguments to be passed to formatC in case of no error, or to format.errors otherwise |

Details

It is strongly recommended to install the errors-package. Otherwise the formatting options are significantly reduced.

The value of the first element of x is properly rounded to its significant digits determined by the values of dx or the second element of x (see above) and digits. Then a tex-ready string is returned.

Value

writes a string to standard output

Author(s)

Carsten Urbach, <curbach@gmx.de> and Johann Ostmeyer

Examples

```
tex.catwitherror(x=0.375567, dx=0.001) tex.catwitherror(x=c(0.375567, 0.001)) ## it can be used with apply x = array(c(0.1187, 0.291, 0.388, 0.011, 0.037, 0.021), dim=c(3,2)) apply(x, 1, tex.catwitherror, digits=2)
```

tikz.finalize

tikz.finalize

Description

initialize and finalize a tikzDevice and carry out optional post-processing

Usage

```
tikz.finalize(tikzfiles, crop = TRUE, margins = 0, clean = TRUE)
```

186 tikz.init

Arguments

tikzfiles a list with members \$pdf, \$tex, \$aux and \$log, returned by tikz.init which

must be passed to tikz.finalize

crop boolean indicating whether pdfcrop should be called on the resulting pdf (ex-

istence of pdfcrop is checked before the command is called), default TRUE

margins margins argument for pdfcrop command, should be passed as a string consisting

of one or multiple numbers (e.g. "10" or "10.5 7.5 6.2 10"), default 0

clean boolean indicating whether temporary files, e.g. "basename.tex", "basename.aux"

and "basename.log" should be deleted after the pdf has been generated, default

TRUE

Details

Convenience Functions for tikzDevice

Value

No return value, but the output PDF will be created and cropped.

Author(s)

Bartosz Kostrzewa, <bartosz.kostrzewa@desy.de>

See Also

```
tikz.init
```

Other tikzutils: tikz.init()

tikz.init

tikz.init

Description

initialize and finalize a tikzDevice and carry out optional post-processing

Usage

```
tikz.init(basename, standAlone = TRUE, engine, ...)
```

Arguments

| basename | the base of the | files which will b | be used by tikzDevice, e.g. | "basename" -> |
|----------|-----------------|--------------------|-----------------------------|---------------|
|----------|-----------------|--------------------|-----------------------------|---------------|

"basename.pdf", etc.

standAlone A logical value indicating whether the output file should be suitable for direct

processing by LaTeX. A value of FALSE indicates that the file is intended for

inclusion in a larger document.

engine used to specify the LaTex engine. If missing, the standard engine of tikz is used.

... optional arguments which are passed to tikz, see tikzDevice::tikz

unsymmetrise.cf 187

Details

Convenience Functions for tikzDevice

Value

tikz.init returns a list with character vector members, \$pdf, \$tex, \$aux \$log containing the corresponding filenames

Author(s)

Bartosz Kostrzewa, <bartosz.kostrzewa@desy.de>

See Also

```
Other tikzutils: tikz.finalize()
```

Examples

```
tikzfiles <- tikz.init("plotname",width=3,height=4)
plot(x=c(1:3), y=c(1:3)^2, xlab="$x$", ylab="$y$")
tikz.finalize(tikzfiles=tikzfiles, clean=TRUE)
file.remove("plotname.pdf")</pre>
```

unsymmetrise.cf

Unfold a correlation function which has been symmetrised

Description

After a symmetric correlation function has been averaged across the central time slice, it is sometimes useful to explicitly duplicate the resulting average to span all cf\$Time time slices. This function takes a cf with cf\$Time/2+1 time slices and turns it into one with cf\$Time time slices by reflecting the correlation function along the cf\$Time/2 axis.

Usage

```
unsymmetrise.cf(cf, sym.vec = c(1))
```

Arguments

cf cf object which has been previously symmetrised

sym.vec Integer vector giving the symmetry properties (see symmetrise.cf) of the original

unsymmetrised correlation function. This should be of length cf\$nrObs

Value

Returns an object of class cf, which is the unfolded version of the input cf object.

188 uwerr

uwerr

Time Series Analysis With Gamma Method

Description

Analyse time series data with the so called gamma method

Usage

```
uwerr(f, data, nrep, S = 1.5, pl = FALSE, ...)
```

Arguments

| f | function computing the derived quantity. If not given it is assumed that a primary quantity is analysed. |
|------|--|
| | f must have the data vector of length Nalpha as the first argument. Further arguments to f can be passed to uwerr via the argument. |
| | f may return a vector object of numeric type. |
| data | array of data to be analysed. It must be of dimension (N x Nalpha) (i.e. N rows and Nalpha columns), where N is the total number of measurements and Nalpha is the number of primary observables |
| nrep | the vector (N1, N2,) of replica length N1, N2 |
| S | initial guess for the ratio tau/tauint, with tau the exponetial autocorrelation length. |
| pl | logical: if TRUE, the autocorrelation function, the integrated autocorrelation time as function of the integration cut-off and (for primary quantities) the time history of the observable are plotted with plot.uwerr |
| | arguments passed to function f. |

Value

In case of a primary observable (uwerrprimary), an object of class uwerr with basis class list containing the following objects

value the expectation value of the obsevable dvalue the error estimate

ddvalue estimate of the error on the error

tauint estimate of the integrated autocorrelation time for that quantity

dtauint error of tauint

Qval the p-value of the weighted average in case of several replicas

In case of a derived observable (uwerrderived), i.e. if a function is specified, the above objects are contained in a list called res.

uwerrprimary returns in addition

data input data

uwerr 189

whereas uwerrderived returns

datamean (vector of) mean(s) of the (vector of) data

and in addition

fgrad the estimated gradient of f

and

f the input statistics

In both cases the return object containes

Wopt value of optimal cut-off for the Gamma function integration

Wmax maximal value of the cut-off for the Gamma function integration

tauintofW integrated autocorrelation time as a function of the cut-off W

dtauintofW error of the integrated autocorrelation time as a function of the cut-off W

S input parameter S

N total number of observations

R number of replicas

nrep vector of observations per replicum

Gamma normalised autocorrelation function

primary set to 1 for uwerrprimary and 0 for uwerrderived

Author(s)

Carsten Urbach, <curbach@gmx.de>

References

"Monte Carlo errors with less errors", Ulli Wolff, Comput.Phys.Commun. 156 (2004) 143-153, Comput.Phys.Commun. 176 (2007) 383 (erratum), hep-lat/0306017

See Also

```
plot.uwerr
```

Examples

```
data(plaq.sample)
plaq.res <- uwerrprimary(plaq.sample)
summary(plaq.res)
plot(plaq.res)</pre>
```

190 uwerr.raw_cf

uwerr.cf

uwerr.cf

Description

Gamma method analysis on all time-slices in a 'cf' object

Usage

```
uwerr.cf(cf)
```

Arguments

cf

Object of type cf containing cf_orig

Value

A list with a named element uwcf which contains a data frame with six columns, value, dvalue, ddvalue, tauint, dtauint corresponding to what is returned by uwerrprimary. The sixth column, t, is just an index counting the columns in the original cf\$cf. If cf contains an imaginary part, the return value contains another list element, uwicf of the same structure as uwcf. There are as many rows as there were columns in cf\$cf and/or cf\$icf. When the call to uwerrprimary fails for a particular column of cf\$cf or cf\$icf, the corresponding row of uwcf and/or uwicf will contain NA for all members.

Examples

```
data(samplecf)
uwerr.cf(samplecf)
```

uwerr.raw_cf

Gamma method analysis on all time-slices in a 'raw_cf' object

Description

Gamma method analysis on all time-slices in a 'raw_cf' object

Usage

```
uwerr.raw_cf(cf)
```

Arguments

cf

Correlation function container of class 'raw_cf'

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Value

The return value is a list with elements

value central value dvalue statistical error

ddvalue error of the statistical error

tauint auto-correlation time estimate

dtauint error of auto-correlation time estimate

Each of these is in turn an array of dimension c(cf\$nts, cf\$dim) and hance lacks the first dimension index compared for cf\$data.

weight.cf

Weight a correlation function

Description

Weights a correlation function with the given energy difference ΔE such that the function is first multiplied with $\exp(\Delta E t) + c \exp(\Delta E \cdot (Time - t))$.

Usage

```
weight.cf(cf, energy_difference_val, energy_difference_boot, cosh_factor,
 offset = 0, inverse = FALSE)
```

Arguments

cf cf_orig and possibly cf_boot object.

energy_difference_val

numeric. A single energy value ΔE for the weighting.

energy_difference_boot

numeric vector. Samples for the energy difference value.

cosh_factor integer, either +1 or -1. Determines the sign \$c\$ in the weight factor. offset

integer. Offset for the time \$t\$, needed for the reweighting after a shift.

inverse boolean. If TRUE apply inverse weight.

Value

Returns an object of class cf, see cf.

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```
weight_shift_reweight.cf
                          Weight-shift-reweight a correlation function
```

Description

The correlation function is weighted with weight.cf, then shifted, and then weighted again with the inverse weighting factor.

Usage

```
weight_shift_reweight.cf(cf, energy_difference_val, energy_difference_boot,
  cosh_factor)
```

Arguments

```
cf
                  cf_orig and possibly cf_boot object.
energy_difference_val
                   numeric. A single energy value \Delta E for the weighting.
energy_difference_boot
                  numeric vector. Samples for the energy difference value.
cosh_factor
                  integer, either +1 or -1. Determines the sign $c$ in the weight factor.
```

Value

Returns an object of class cf, see cf.

zetazp

Computes the running of Z_P from scale mu0 to scale mu2

Description

Computes the running of the renomalisation constant Z_P from scale μ_0 to scale μ_2 in the renomalisation schema RI' for $N_f = 2$ only. The running is done using perturbation theory up to $\alpha_s **3$ order. The corresponding values of α_s at the scales μ_0 and μ_2 are needed as input, see alphas.

Usage

```
zetazp(zp0, alpha0, alpha2, nl = 3)
```

Arguments

nl

```
zp0
                      initial value of Z_P
alpha0
                      \alpha_s at initial scale
alpha2
                      \alpha_s at final scale
                      order in PT, range 0 to 3
```

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Value

returns the value of Z_P at scale mu2 in the RI' scheme

Author(s)

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See Also

alphas

Examples

```
al2 <- alphas(mu = 3.0, nl = 3, lam0 = 0.250, Nc = 3, Nf = 2) al0 <- alphas(mu = 2.0, nl = 3, lam0 = 0.250, Nc = 3, Nf = 2) zetazp(zp0 = 0.6, alpha0 = al0, alpha2 = al2, nl = 3)
```

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