Package: AIUQ (via r-universe)

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Type Package

Title Ab Initio Uncertainty Quantification

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Description Uncertainty quantification and inverse estimation by probabilistic generative models from the beginning of the data analysis. An example is a Fourier basis method for inverse estimation in scattering analysis of microscopy videos. It does not require specifying a certain range of Fourier bases and it substantially reduces computational cost via the generalized Schur algorithm. See the reference: Mengyang Gu, Yue He, Xubo Liu and Yimin Luo (2023), <doi:10.48550/arXiv.2309.02468>.

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Imports fftwtools (>= 0.9.11), SuperGauss (>= 2.0.3), methods, plot3D (>= 1.4)

NeedsCompilation no

Suggests knitr, rmarkdown

VignetteBuilder knitr

Repository CRAN

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Contents

`aniso_SAM` *Scattering analysis of microscopy for anisotropic processes*

Description

Fast parameter estimation in scattering analysis of microscopy for anisotropic processes, using AIUQ method.

Usage

```
aniso_SAM(
  intensity = NA,
  intensity_str = "T_SS_mat",
  pxsz = 1,
  sz = c(NA, NA),
  mindt = 1,
  AIUQ_thr = c(1, 1),
  model_name = "BM",
  sigma_0_2_ini = NaN,
  param_initial = NA,
  num_optim = 1,
  msd_fn = NA,
  msd_grad_fn = NA,
  num_param = NA,
  uncertainty = FALSE,
  M = 50,
  sim_object = NA,
  msd_truth = NA,
  method = "AIUQ",
  index_q_AIUQ = NA,
  message_out = TRUE,
```

```
  square = FALSE
)
```

Arguments

- `intensity` — intensity profile. See 'Details'.
- `intensity_str` — structure of the intensity profile, options from ('SST_array','S_ST_mat','T_SS_mat'). See 'Details'.
- `pxsz` — size of one pixel in unit of micron, 1 for simulated data
- `sz` — frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.
- `mindt` — minimum lag time, 1 for simulated data
- `AIUQ_thr` — threshold for wave number selection, numeric vector of two elements with values between 0 and 1. See 'Details'.
- `model_name` — fitted model, options from ('BM','OU','FBM','OU+FBM', 'user_defined'), with Brownian motion as the default model. See 'Details'.
- `sigma_0_2_ini` — initial value for background noise. If NA, use minimum value of absolute square of intensity profile in reciprocal space.
- `param_initial` — initial values for param estimation.
- `num_optim` — number of optimization.
- `msd_fn` — user defined mean squared displacement(MSD) structure, a function of parameters and lag times. NA if `model_name` is not 'user_defined'.
- `msd_grad_fn` — gradient for user defined mean squared displacement structure. If `NA`, then numerical gradient will be used for parameter estimation in `'user_defined'` model.
- `num_param` — number of parameters need to be estimated in the intermediate scattering function, need to be non-NA value for user_defined' model.
- `uncertainty` — a logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.
- `M` — number of particles. See 'Details'.
- `sim_object` — NA or an S4 object of class `simulation`.
- `msd_truth` — true MSD or reference MSD value.
- `method` — methods for parameter estimation, options from ('AIUQ', 'DDM').
- `index_q_AIUQ` — index range for wave number when using AIUQ method. See 'Details'.
- `message_out` — a logical evaluating to TRUE or FALSE indicating whether or not to output the message.
- `square` — a logical evaluating to TRUE or FALSE indicating whether or not to crop the original intensity profile into square image.

Details

For simulated data using `aniso_simulation` in AIUQ package, `intensity` will be automatically extracted from `aniso_simulation` class.

By default `intensity_str` is set to 'T_SS_mat', a time by space×space matrix, which is the structure of intensity profile obtained from `aniso_simulation` class. For `intensity_str='SST_array'` , input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by space×time matrix.

By default `AIUQ_thr` is set to `c(1,1)`, uses information from all complete q rings. The first element affects maximum wave number selected, and second element controls minimum proportion of wave number selected. By setting 1 for the second element, if maximum wave number selected is less than the wave number length, then maximum wave number selected is coerced to use all wave number unless user defined another index range through `index_q_AIUQ`.

If `model_name` equals 'user_defined', or NA (will coerced to 'user_defined'), then `msd_fn` and `num_param` need to be provided for parameter estimation.

Number of particles `M` is set to 50 or automatically extracted from `simulation` class for simulated data using `simulation` in AIUQ package.

By default, using all wave vectors from complete q ring for both `AIUQ`, unless user defined index range through `index_q_AIUQ`.

Value

Returns an S4 object of class `aniso_SAM`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
# Example 1: Estimation for simulated data
set.seed(1)
aniso_sim = aniso_simulation(sz=100,len_t=100, model_name="BM",M=100,sigma_bm=c(0.5,0.3))
show(aniso_sim)
plot_traj(object=aniso_sim)
aniso_sam = aniso_SAM(sim_object=aniso_sim, model_name="BM",AIUQ_thr = c(0.999,0))
show(aniso_sam)
plot_MSD(aniso_sam,msd_truth = aniso_sam@msd_truth)
```

aniso_SAM-class *Anisotropic SAM class*

Description

S4 class for fast parameter estimation in scattering analysis of microscopy for anisotropic processes, using either AIUQ or DDM method.

Slots

- `pxsz` numeric. Size of one pixel in unit of micron with default value 1.
- `mindt` numeric. Minimum lag time with default value 1.
- `sz` vector. Frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.
- `len_t` integer. Number of time steps.
- `len_q` integer. Number of wave vector.
- `q` vector. Wave vector in unit of um^-1.
- `d_input` vector. Sequence of lag times.
- `B_est_ini` numeric. Estimation of B. This parameter is determined by the noise in the system. See 'References'.
- `A_est_ini` vector. Estimation of A(q). Note this parameter is determined by the properties of the imaged material and imaging optics. See 'References'.
- `I_o_q_2_ori` vector. Absolute square of Fourier transformed intensity profile, ensemble over time.
- `q_ori_ring_loc_unique_index` list. List of location index of non-duplicate values for each q ring.
- `model_name` character. Fitted model, options from ('BM','OU','FBM','OU+FBM', 'user_defined').
- `param_est` matrix. Estimated parameters contained in MSD.
- `sigma_2_0_est` vector. Estimated variance of background noise.
- `msd_est` matrix. Estimated MSD.
- `uncertainty` logical. A logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.
- `msd_truth` matrix. True MSD or reference MSD value.
- `sigma_2_0_truth` vector. True variance of background noise, non NA for simulated data using `simulation`.
- `param_truth` matrix. True parameters used to construct MSD, non NA for simulated data using `aniso_simulation`.
- `index_q` vector. Selected index of wave vector.
- `I_q` matrix. Fourier transformed intensity profile with structure 'SS_T_mat'.
- `AIC` numeric. Akaike information criterion score.
- `mle` numeric. Maximum log likelihood value.

`msd_x_lower` vector. Lower bound of 95% confidence interval of MSD in x directions.

`msd_x_upper` vector. Upper bound of 95% confidence interval of MSD in x directions.

`msd_y_lower` vector. Lower bound of 95% confidence interval of MSD in y directions.

`msd_y_upper` vector. Upper bound of 95% confidence interval of MSD in y directions.

`param_uq_range` matrix. 95% confidence interval for estimated parameters.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

`aniso_simulation` *Simulate anisotropic 2D particle movement*

Description

Simulate anisotropic 2D particle movement from a user selected stochastic process, and output intensity profiles.

Usage

```
aniso_simulation(
  sz = c(200, 200),
  len_t = 200,
  M = 50,
  model_name = "BM",
  noise = "gaussian",
  I0 = 20,
  Imax = 255,
  pos0 = matrix(NaN, nrow = M, ncol = 2),
  rho = c(0.95, 0.9),
  H = c(0.4, 0.3),
  sigma_p = 2,
  sigma_bm = c(1, 0.5),
  sigma_ou = c(2, 1.5),
  sigma_fbm = c(2, 1.5)
)
```

Arguments

sz	frame size of simulated image with default `c(200,200)`.
len_t	number of time steps with default 200.
M	number of particles with default 50.
model_name	stochastic process simulated, options from ('BM','OU','FBM','OU+FBM'), with default 'BM'.
noise	background noise, options from ('uniform','gaussian'), with default 'gaussian'.
I0	background intensity, value between 0 and 255, with default 20.
Imax	maximum intensity at the center of the particle, value between 0 and 255, with default 255.
pos0	initial position for M particles, matrix with dimension M by 2.
rho	correlation between successive step and previous step in O-U process, in x, y-directions. A vector of length 2 with values between 0 and 1, default `c(0.95,0.9)`.
H	Hurst parameter of fractional Brownian Motion, in x, y-directions. A vector of length 2, value between 0 and 1, default `c(0.4,0.3)`.
sigma_p	radius of the spherical particle (3sigma_p), with default 2.
sigma_bm	distance moved per time step of Brownian Motion, in x,y-directions. A vector of length 2 with default `c(1,0.5)`.
sigma_ou	distance moved per time step of Ornstein–Uhlenbeck process, in x, y-directions. A vector of length 2 with default `c(2,1.5)`.
sigma_fbm	distance moved per time step of fractional Brownian Motion, in x, y-directions. A vector of length 2 with default `c(2,1.5)`.

Value

Returns an S4 object of class `anisotropic_simulation`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
# --------------------------------------------------
# Example 1: Simple diffusion for 200 images with
#            200 by 200 pixels and 50 particles
# --------------------------------------------------
aniso_sim_bm = aniso_simulation()
show(aniso_sim_bm)

# --------------------------------------------------
# Example 2: Simple diffusion for 100 images with
#            100 by 100 pixels and slower speed
# --------------------------------------------------
aniso_sim_bm = aniso_simulation(sz=100,len_t=100,sigma_bm=c(0.5,0.1))
show(aniso_sim_bm)

# --------------------------------------------------
# Example 3: Ornstein-Uhlenbeck process
# --------------------------------------------------
aniso_sim_ou = aniso_simulation(model_name="OU")
show(aniso_sim_ou)
```

---

aniso_simulation-class *Anisotropic simulation class*

Description

S4 class for anisotropic 2D particle movement simulation.

Details

intensity should has structure 'T_SS_mat', matrix with dimension len_t by sz×sz.

pos should be the position matrix with dimension M×len_t. See bm_particle_intensity, ou_particle_intensity, fbm_particle_intensity, fbm_ou_particle_intensity.

Slots

sz vector. Frame size of the intensity profile, number of pixels contained in each frame equals sz[1] by sz[2].

len_t integer. Number of time steps.

noise character. Background noise, options from ('uniform','gaussian').

model_name character. Simulated stochastic process, options from ('BM','OU','FBM','OU+FBM').

M integer. Number of particles.

pxsz numeric. Size of one pixel in unit of micron, 1 for simulated data.

mindt numeric. Minimum lag time, 1 for simulated data.

`pos` matrix. Position matrix for particle trajectory, see 'Details'.

`intensity` matrix. Filled intensity profile, see 'Details'.

`num_msd` matrix. Numerical mean squared displacement (MSD).

`param` matrix. Parameters used to construct MSD.

`theor_msd` matrix. Theoretical MSD.

`sigma_2_0` vector. Variance of background noise.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

---

get_dqt *Compute observed dynamic image structure function*

Description

Compute observed dynamic image structure function (Dqt) using object of `SAM` class.

Usage

```
get_dqt(object, index_q = NA)
```

Arguments

`object`	an S4 object of class `SAM`
`index_q`	wavevector range used for computing Dqt

Value

A matrix of observed dynamic image structure function with dimension `len_q` by `len_t-1`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
## Not run:
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
Dqt = get_dqt(object=sam)

## End(Not run)
```

---

get_isf — *Compute empirical intermediate scattering function*

Description

Compute empirical intermediate scattering function (ISF) using object of `SAM` class.

Usage

```
get_isf(object, index_q = NA, msd_truth = NA)
```

Arguments

`object`	an S4 object of class `SAM`
`index_q`	wavevector range used for computing ISF
`msd_truth`	true or reference MSD

Value

A matrix of empirical intermediate scattering function with dimension `len_q` by `len_t-1`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
## Not run:
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
ISF = get_isf(object=sam)

## End(Not run)
```

---

modeled_dqt — *Compute modeled dynamic image structure function*

Description

Compute modeled dynamic image structure function (Dqt) using object of `SAM` class.

Usage

```
modeled_dqt(object, index_q = NA, uncertainty = FALSE)
```

Arguments

`object`	an S4 object of class `SAM`
`index_q`	wavevector range used for computing Dqt
`uncertainty`	logic evalution

Value

A matrix of modeled dynamic image structure function with dimension `len_q` by `len_t-1`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
modeled_Dqt = modeled_dqt(object=sam)
```

---

modeled_isf   *Compute modeled intermediate scattering function*

Description

Compute modeled intermediate scattering function (ISF) using object of `SAM` class.

Usage

```
modeled_isf(object, index_q = NA)
```

Arguments

`object`	an S4 object of class `SAM`
`index_q`	wavevector range used for computing ISF

Value

A matrix of modeled intermediate scattering function with dimension `len_q` by `len_t-1`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
modeled_ISF = modeled_isf(object=sam)
```

`plot_intensity` *Plot 2D intensity*

Description

Function to plot 2D intensity profile for a certain frame, default is to plot the first frame. Input can be a matrix (2D) or an array (3D).

Usage

```
plot_intensity(
  intensity,
  intensity_str = "T_SS_mat",
  frame = 1,
  sz = NA,
  title = NA,
  color = FALSE
)
```

Arguments

`intensity`	intensity profile
`intensity_str`	structure of the intensity profile, options from ('SST_array','S_ST_mat','T_SS_mat', 'SS_T_mat'). See 'Details'.
`frame`	frame index
`sz`	frame size of simulated image with default `c(200,200)`.
`title`	main title of the plot. If `NA`, title is "intensity profile for frame n" with n being the frame index in `frame`.
`color`	a logical evaluating to TRUE or FALSE indicating whether a colorful plot is generated

Details

By default `intensity_str` is set to 'T_SS_mat', a time by space×space matrix, which is the structure of intensity profile obtained from `simulation` class. For `intensity_str='SST_array'` , input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by space×time matrix. For `intensity_str='SS_T_mat'`, input intensity profile should be a space×space by time matrix.

Value

2D plot in gray scale (or with color) of selected frame.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

Examples

```
library(AIUQ)
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)
plot_intensity(sim_bm@intensity, sz=sim_bm@sz)
```

---

plot_MSD *Plot estimated MSD with uncertainty from SAM class*

Description

Function to plot estimated MSD with uncertainty from `SAM` class, versus true mean squared displacement(MSD) or given reference values.

Usage

```
plot_MSD(object, msd_truth = NA, title = NA, log10 = TRUE)
```

Arguments

`object`	an S4 object of class `SAM`
`msd_truth`	a vector/matrix of true MSD or reference MSD value, default is `NA`
`title`	main title of the plot. If `NA`, title is "model_name" with `model_name` being a field in `SAM` class representing fitted model.
`log10`	a logical evaluating to TRUE or FALSE indicating whether a plot in log10 scale is generated

Value

A plot of estimated MSD with uncertainty versus truth/reference values.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Examples

```
library(AIUQ)

## Simulate BM and get estimated parameters with uncertainty using BM model
# Simulation
set.seed(1)
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)

# AIUQ method: fitting using BM model
sam = SAM(sim_object=sim_bm, uncertainty=TRUE,AIUQ_thr=c(0.999,0))
show(sam)

plot_MSD(object=sam, msd_truth=sam@msd_truth) #in log10 scale
plot_MSD(object=sam, msd_truth=sam@msd_truth,log10=FALSE) #in real scale
```

---

plot_traj — *Plot 2D particle trajectory*

Description

Function to plot the particle trajectory after the `simulation` class has been constructed.

Usage

```
plot_traj(object, title = NA)
```

Arguments

`object`	an S4 object of class `simulation`
`title`	main title of the plot. If `NA`, title is "model_name with M particles" with `model_name` and `M` being field in `simulation` class.

Value

2D plot of particle trajectory for a given simulation from `simulation` class.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

Examples

```
library(AIUQ)
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)
plot_traj(sim_bm)
```

SAM *Scattering analysis of microscopy*

Description

Fast parameter estimation in scattering analysis of microscopy, using either AIUQ or DDM method.

Usage

```
SAM(
  intensity = NA,
  intensity_str = "T_SS_mat",
  pxsz = 1,
  sz = c(NA, NA),
  mindt = 1,
  AIUQ_thr = c(1, 1),
  model_name = "BM",
  sigma_0_2_ini = NaN,
  param_initial = NA,
  num_optim = 1,
  msd_fn = NA,
  msd_grad_fn = NA,
  num_param = NA,
  uncertainty = FALSE,
  M = 50,
  sim_object = NA,
  msd_truth = NA,
  method = "AIUQ",
  index_q_AIUQ = NA,
  index_q_DDM = NA,
  message_out = TRUE,
  A_neg = "abs",
  square = FALSE,
  output_dqt = FALSE,
  output_isf = FALSE,
  output_modeled_isf = FALSE,
  output_modeled_dqt = FALSE
)
```

Arguments

`intensity`	intensity profile. See 'Details'.
`intensity_str`	structure of the intensity profile, options from ('SST_array','S_ST_mat','T_SS_mat'). See 'Details'.
`pxsz`	size of one pixel in unit of micron, 1 for simulated data
`sz`	frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.
`mindt`	minimum lag time, 1 for simulated data
`AIUQ_thr`	threshold for wave number selection, numeric vector of two elements with values between 0 and 1. See 'Details'.
`model_name`	fitted model, options from ('BM','OU','FBM','OU+FBM', 'user_defined'), with Brownian motion as the default model. See 'Details'.
`sigma_0_2_ini`	initial value for background noise. If NA, use minimum value of absolute square of intensity profile in reciprocal space.
`param_initial`	initial values for param estimation.
`num_optim`	number of optimization.
`msd_fn`	user defined mean squared displacement(MSD) structure, a function of parameters and lag times. NA if `model_name` is not 'user_defined'.
`msd_grad_fn`	gradient for user defined mean squared displacement structure. If `NA`, then numerical gradient will be used for parameter estimation in `'user_defined'` model.
`num_param`	number of parameters need to be estimated in the intermediate scattering function, need to be non-NA value for user_defined' model.
`uncertainty`	a logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.
`M`	number of particles. See 'Details'.
`sim_object`	NA or an S4 object of class `simulation`.
`msd_truth`	true MSD or reference MSD value.
`method`	methods for parameter estimation, options from ('AIUQ','DDM_fixedAB','DDM_estAB').
`index_q_AIUQ`	index range for wave number when using AIUQ method. See 'Details'.
`index_q_DDM`	index range for wave number when using DDM method. See 'Details'.
`message_out`	a logical evaluating to TRUE or FALSE indicating whether or not to output the message.
`A_neg`	controls modification for negative A(q), options from ('abs','zero'), with setting negative A(q) to its absolute value as the default.
`square`	a logical evaluating to TRUE or FALSE indicating whether or not to crop the original intensity profile into square image.
`output_dqt`	a logical evaluating to TRUE or FALSE indicating whether or not to compute observed dynamic image structure function(Dqt).
`output_isf`	a logical evaluating to TRUE or FALSE indicating whether or not to compute empirical intermediate scattering function(ISF).

`output_modeled_isf`
: a logical evaluating to TRUE or FALSE indicating whether or not to compute modeled intermediate scattering function(ISF).

`output_modeled_dqt`
: a logical evaluating to TRUE or FALSE indicating whether or not to compute modeled dynamic image structure function(Dqt).

Details

For simulated data using `simulation` in AIUQ package, `intensity` will be automatically extracted from `simulation` class.

By default `intensity_str` is set to 'T_SS_mat', a time by space$\times$space matrix, which is the structure of intensity profile obtained from `simulation` class. For `intensity_str='SST_array'` , input intensity profile should be a space by space by time array, which is the structure from loading a tif file. For `intensity_str='S_ST_mat'`, input intensity profile should be a space by space$\times$time matrix.

By default `AIUQ_thr` is set to `c(1,1)`, uses information from all complete q rings. The first element affects maximum wave number selected, and second element controls minimum proportion of wave number selected. By setting 1 for the second element, if maximum wave number selected is less than the wave number length, then maximum wave number selected is coerced to use all wave number unless user defined another index range through `index_q_AIUQ`.

If `model_name` equals 'user_defined', or NA (will coerced to 'user_defined'), then `msd_fn` and `num_param` need to be provided for parameter estimation.

Number of particles `M` is set to 50 or automatically extracted from `simulation` class for simulated data using `simulation` in AIUQ package.

By default, using all wave vectors from complete q ring, unless user defined index range through `index_q_AIUQ` or `index_q_DDM`.

Value

Returns an S4 object of class `SAM`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
# Example 1: Estimation for simulated data
sim_bm = simulation(len_t=100,sz=100,sigma_bm=0.5)
show(sim_bm)
sam = SAM(sim_object = sim_bm)
show(sam)
```

SAM-class *SAM class*

Description

S4 class for fast parameter estimation in scattering analysis of microscopy, using either `AIUQ` or `DDM` method.

Slots

`pxsz` numeric. Size of one pixel in unit of micron with default value 1.

`mindt` numeric. Minimum lag time with default value 1.

`sz` vector. Frame size of the intensity profile in x and y directions, number of pixels contained in each frame equals sz_x by sz_y.

`len_t` integer. Number of time steps.

`len_q` integer. Number of wave vector.

`q` vector. Wave vector in unit of um^-1.

`d_input` vector. Sequence of lag times.

`B_est_ini` numeric. Estimation of B. This parameter is determined by the noise in the system. See 'References'.

`A_est_ini` vector. Estimation of A(q). Note this parameter is determined by the properties of the imaged material and imaging optics. See 'References'.

`I_o_q_2_ori` vector. Absolute square of Fourier transformed intensity profile, ensemble over time.

`q_ori_ring_loc_unique_index` list. List of location index of non-duplicate values for each q ring.

`model_name` character. Fitted model, options from ('BM','OU','FBM','OU+FBM', 'user_defined').

`param_est` vector. Estimated parameters contained in MSD.

`sigma_2_0_est` numeric. Estimated variance of background noise.

`msd_est` vector. Estimated MSD.

`uncertainty` logical. A logical evaluating to TRUE or FALSE indicating whether parameter uncertainty should be computed.

`msd_lower` vector. Lower bound of 95% confidence interval of MSD.

`msd_upper` vector. Upper bound of 95% confidence interval of MSD.

msd_truth vector. True MSD or reference MSD value.

sigma_2_0_truth vector. True variance of background noise, non NA for simulated data using simulation.

param_truth vector. True parameters used to construct MSD, non NA for simulated data using simulation.

index_q vector. Selected index of wave vector.

Dqt matrix. Dynamic image structure function D(q,delta t).

ISF matrix. Empirical intermediate scattering function f(q,delta t).

I_q matrix. Fourier transformed intensity profile with structure 'SS_T_mat'.

AIC numeric. Akaike information criterion score.

mle numeric. Maximum log likelihood value.

param_uq_range matrix. 95% confidence interval for estimated parameters.

modeled_Dqt matrix. Modeled dynamic image structure function D(q,delta t).

modeled_ISF matrix. Modeled intermediate scattering function f(q,delta t).

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

---

show.aniso_sam *Show scattering analysis of microscopy for anisotropic processes (aniso_SAM) object*

Description

Function to print the aniso_SAM class object after the aniso_SAM model has been constructed.

Usage

```
show.aniso_sam(object)
```

Arguments

object	an S4 object of class aniso_SAM

Value

Show a list of important parameters in class aniso_SAM.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Examples

```
library(AIUQ)

## Simulate BM and get estimated parameters using BM model
# Simulation
aniso_sim_bm = aniso_simulation(sz=100,len_t=100,sigma_bm=c(0.5,0.3))
show(aniso_sim_bm)

# AIUQ method: fitting using BM model
aniso_sam = aniso_SAM(sim_object=aniso_sim_bm, AIUQ_thr=c(0.99,0))
show(aniso_sam)
```

---

show.aniso_simulation *Show anisotropic simulation object*

Description

Function to print the aniso_simulation class object after the aniso_simulation model has been constructed.

Usage

```
show.aniso_simulation(object)
```

Arguments

object	an S4 object of class aniso_simulation

Value

Show a list of important parameters in class aniso_simulation.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Examples

```
library(AIUQ)

# Simulate simple diffusion for 100 images with 100 by 100 pixels
aniso_sim_bm = aniso_simulation(sz=100,len_t=100,sigma_bm=c(0.5,0.1))
show(aniso_sim_bm)
```

---

show.sam   *Show scattering analysis of microscopy (SAM) object*

Description

Function to print the `SAM` class object after the `SAM` model has been constructed.

Usage

```
show.sam(object)
```

Arguments

`object`	an S4 object of class `SAM`

Value

Show a list of important parameters in class `SAM`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Examples

```
library(AIUQ)

## Simulate BM and get estimated parameters using BM model
# Simulation
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)

# AIUQ method: fitting using BM model
sam = SAM(sim_object=sim_bm)
show(sam)
```

`show.simulation` *Show simulation object*

Description

Function to print the `simulation` class object after the `simulation` model has been constructed.

Usage

```
show.simulation(object)
```

Arguments

`object`	an S4 object of class `simulation`

Value

Show a list of important parameters in class `simulation`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Examples

```
library(AIUQ)

# Simulate simple diffusion for 100 images with 100 by 100 pixels
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)
```

simulation *Simulate 2D particle movement*

Description

Simulate 2D particle movement from a user selected stochastic process, and output intensity profiles.

Usage

```
simulation(
  sz = c(200, 200),
  len_t = 200,
  M = 50,
  model_name = "BM",
  noise = "gaussian",
  I0 = 20,
  Imax = 255,
  pos0 = matrix(NaN, nrow = M, ncol = 2),
  rho = 0.95,
  H = 0.3,
  sigma_p = 2,
  sigma_bm = 1,
  sigma_ou = 2,
  sigma_fbm = 2
)
```

Arguments

sz	frame size of simulated image with default c(200,200).
len_t	number of time steps with default 200.
M	number of particles with default 50.
model_name	stochastic process simulated, options from ('BM','OU','FBM','OU+FBM'), with default 'BM'.
noise	background noise, options from ('uniform','gaussian'), with default 'gaussian'.
I0	background intensity, value between 0 and 255, with default 20.
Imax	maximum intensity at the center of the particle, value between 0 and 255, with default 255.
pos0	initial position for M particles, matrix with dimension M by 2.
rho	correlation between successive step and previous step in O-U process, value between 0 and 1, with default 0.95.
H	Hurst parameter of fractional Brownian Motion, value between 0 and 1, with default 0.3.
sigma_p	radius of the spherical particle (3sigma_p), with default 2.

sigma_bm	distance moved per time step in Brownian Motion, with default 1.
sigma_ou	distance moved per time step in Ornstein–Uhlenbeck process, with default 2.
sigma_fbm	distance moved per time step in fractional Brownian Motion, with default 2.

Value

Returns an S4 object of class `simulation`.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

Examples

```
library(AIUQ)
# -------------------------------------------------
# Example 1: Simple diffusion for 200 images with
#            200 by 200 pixels and 50 particles
# -------------------------------------------------
sim_bm = simulation()
show(sim_bm)

# -------------------------------------------------
# Example 2: Simple diffusion for 100 images with
#            100 by 100 pixels and slower speed
# -------------------------------------------------
sim_bm = simulation(sz=100,len_t=100,sigma_bm=0.5)
show(sim_bm)

# -------------------------------------------------
# Example 3: Ornstein-Uhlenbeck process
# -------------------------------------------------
sim_ou = simulation(model_name="OU")
show(sim_ou)
```

simulation-class *Simulation class*

Description

S4 class for 2D particle movement simulation.

Details

intensity should has structure 'T_SS_mat', matrix with dimension len_t by sz×sz.

pos should be the position matrix with dimension M×len_t. See bm_particle_intensity, ou_particle_intensity, fbm_particle_intensity, fbm_ou_particle_intensity.

Slots

sz vector. Frame size of the intensity profile, number of pixels contained in each frame equals sz[1] by sz[2].

len_t integer. Number of time steps.

noise character. Background noise, options from ('uniform','gaussian').

model_name character. Simulated stochastic process, options from ('BM','OU','FBM','OU+FBM').

M integer. Number of particles.

pxsz numeric. Size of one pixel in unit of micron, 1 for simulated data.

mindt numeric. Minimum lag time, 1 for simulated data.

pos matrix. Position matrix for particle trajectory, see 'Details'.

intensity matrix. Filled intensity profile, see 'Details'.

num_msd vector. Numerical mean squared displacement (MSD).

param vector. Parameters for simulated stochastic process.

theor_msd vector. Theoretical MSD.

sigma_2_0 vector. Variance of background noise.

Author(s)

Yue He [aut], Xubo Liu [aut], Mengyang Gu [aut, cre]

References

Gu, M., He, Y., Liu, X., & Luo, Y. (2023). Ab initio uncertainty quantification in scattering analysis of microscopy. arXiv preprint arXiv:2309.02468.

Gu, M., Luo, Y., He, Y., Helgeson, M. E., & Valentine, M. T. (2021). Uncertainty quantification and estimation in differential dynamic microscopy. Physical Review E, 104(3), 034610.

Cerbino, R., & Trappe, V. (2008). Differential dynamic microscopy: probing wave vector dependent dynamics with a microscope. Physical review letters, 100(18), 188102.

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