
fdasrsf Documentation

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A python package for functional data analysis using the square root slope framework and curves using the square root velocity framework which performs pair-wise and group-wise alignment as well as modeling using functional component analysis and regression.

FUNCTIONAL ALIGNMENT

Group-wise function alignment using SRSF framework and Dynamic Programming

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`time_warping.align_fPCA(f, time, num_comp=3, showplot=True, smoothdata=False)`

aligns a collection of functions while extracting principal components. The functions are aligned to the principal components

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **num_comp** – number of fPCA components
- **showplot** – Shows plots of results using matplotlib (default = T)
- **smooth_data** (*bool*) – Smooth the data using a box filter (default = F)
- **sparam** (*double*) – Number of times to run box filter (default = 25)

Return type tuple of numpy array

Return fn aligned functions - numpy ndarray of shape (M,N) of N functions with M samples

Return qn aligned srvfs - similar structure to fn

Return q0 original srvf - similar structure to fn

Return mqn srvf mean or median - vector of length M

Return gam warping functions - similar structure to fn

Return q_pca srsf principal directions

Return f_pca functional principal directions

Return latent latent values

Return coef coefficients

Return U eigenvectors

Return orig_var Original Variance of Functions

Return amp_var Amplitude Variance

Return phase_var Phase Variance

`time_warping.align_fPLS(f, g, time, comps=3, showplot=True, smoothdata=False, delta=0.01, max_itr=100)`

This function aligns a collection of functions while performing principal least squares

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **g** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **comps** – number of fPLS components
- **showplot** – Shows plots of results using matplotlib (default = T)
- **smooth_data** (*bool*) – Smooth the data using a box filter (default = F)
- **delta** – gradient step size
- **max_itr** – maximum number of iterations

Return type tuple of numpy array

Return fn aligned functions - numpy ndarray of shape (M,N) of N

functions with M samples :return gn: aligned functions - numpy ndarray of shape (M,N) of N functions with M samples :return qfn: aligned srvfs - similar structure to fn :return qgn: aligned srvfs - similar structure to fn :return qf0: original srvf - similar structure to fn :return qg0: original srvf - similar structure to fn :return gam: warping functions - similar structure to fn :return wqf: srsf principal weight functions :return wqg: srsf principal weight functions :return wf: srsf principal weight functions :return wg: srsf principal weight functions :return cost: cost function value

class `time_warping.fdawarp(f, time)`

This class provides alignment methods for functional data using the SRVF framework

Usage: `obj = fdawarp(f,t)`

Parameters

- **f** – (M,N): matrix defining N functions of M samples
- **time** – time vector of length M
- **fn** – aligned functions
- **qn** – aligned srvfs
- **q0** – initial srvfs
- **fmean** – function mean
- **mqn** – mean srvf
- **gam** – warping functions
- **psi** – srvf of warping functions
- **stats** – alignment statistics
- **qun** – cost function
- **lambda** – lambda
- **method** – optimization method
- **gamI** – invserse warping function
- **rsamps** – random samples
- **fs** – random aligned functions
- **gams** – random warping functions

- **ft** – random warped functions
- **qs** – random aligned srvfs
- **type** – alignment type
- **mcmc** – mcmc output if bayesian

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 15-Mar-2018

gauss_model (*n=1, sort_samples=False*)

This function models the functional data using a Gaussian model extracted from the principal components of the srvfs

Parameters

- **n** (*integer*) – number of random samples
- **sort_samples** (*bool*) – sort samples (default = T)

Return type fdawarp object containing

Return fs random aligned samples

Return gams random warping functions

Return ft random samples

joint_gauss_model (*n=1, no=3*)

This function models the functional data using a joint Gaussian model extracted from the principal components of the srsfs

Parameters

- **n** (*integer*) – number of random samples
- **no** (*integer*) – number of principal components (default = 3)

Return type fdawarp object containing

Return fs random aligned samples

Return gams random warping functions

Return ft random samples

plot ()

plot plot functional alignment results

Usage: obj.plot()

srsf_align (*method='mean', omethod='DP', smoothdata=False, parallel=False, lam=0.0*)

This function aligns a collection of functions using the elastic square-root slope (srsf) framework.

Parameters

- **method** – (string) warp calculate Karcher Mean or Median (options = “mean” or “median”) (default=“mean”)
- **omethod** – optimization method (DP, DP2, RBFSGS) (default = DP)
- **smoothdata** (*bool*) – Smooth the data using a box filter (default = F)
- **parallel** – run in parallel (default = F)
- **lam** (*double*) – controls the elasticity (default = 0)

Return type fdawarp obj with fields

Return fn aligned functions - numpy ndarray of shape (M,N) of N

functions with M samples :return qn: aligned srvfs - similar structure to fn :return q0: original srvf - similar structure to fn :return fmean: function mean or median - vector of length M :return mqn: srvf mean or median - vector of length M :return gam: warping functions - similar structure to fn :return orig_var: Original Variance of Functions :return amp_var: Amplitude Variance :return phase_var: Phase Variance

Examples >>> import tables >>> fun=tables.open_file("../Data/simu_data.h5") >>> f = fun.root.f[:] >>> f = f.transpose() >>> time = fun.root.time[:] >>> obj = fs.fdawarp(f,time) >>> obj.srsf_align()

FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS

Vertical and Horizontal Functional Principal Component Analysis using SRSF

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

class `fPCA.fdahpca` (*fdawarp*)

This class provides horizontal fPCA using the SRVF framework

Usage: `obj = fdahpca(warp_data)`

Parameters

- **warp_data** – fdawarp class with alignment data
- **gam_pca** – warping functions principal directions
- **psi_pca** – srvf principal directions
- **latent** – latent values
- **U** – eigenvectors
- **coef** – coefficients
- **vec** – shooting vectors
- **mu** – Karcher Mean
- **tau** – principal directions

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 15-Mar-2018

calc_fpca (*no=3*)

This function calculates horizontal functional principal component analysis on aligned data

Parameters **no** (*int*) – number of components to extract (default = 3)

Return type fdahpca object of numpy ndarray

Return q_pca srsf principal directions

Return f_pca functional principal directions

Return latent latent values

Return coef coefficients

Return U eigenvectors

plot ()

plot plot elastic horizontal fPCA results

Usage: `obj.plot()`

class `fPCA.fdajpca` (*fdawarp*)

This class provides joint fPCA using the SRVF framework

Usage: `obj = fdajpca(warp_data)`

Parameters

- **warp_data** – fdawarp class with alignment data
- **q_pca** – srvf principal directions
- **f_pca** – f principal directions
- **latent** – latent values
- **coef** – principl coefficients
- **id** – point used for $f(0)$
- **mqn** – mean srvf
- **U** – eigenvectors
- **mu_psi** – mean psi
- **mu_g** – mean g
- **C** – scaling value
- **stds** – geodesic directions

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 18-Mar-2018

calc_fpca (*no=3, id=None*)

This function calculates joint functional principal component analysis on aligned data

Parameters

- **no** (*int*) – number of components to extract (default = 3)
- **id** (*int*) – point to use for $f(0)$ (default = midpoint)

Return type fdajpca object of numpy ndarray

Return q_pca srsf principal directions

Return f_pca functional principal directions

Return latent latent values

Return coef coefficients

Return U eigenvectors

plot ()

plot plot elastic vertical fPCA result

Usage: `obj.plot()`

class `fPCA.fdavpca` (*fdawarp*)

This class provides vertical fPCA using the SRVF framework

Usage: `obj = fdavpca(warp_data)`

Parameters

- **warp_data** – fdawarp class with alignment data
- **q_pca** – srvf principal directions

- **f_pca** – f principal directions
- **latent** – latent values
- **coef** – principal coefficients
- **id** – point used for $f(0)$
- **mqn** – mean srvf
- **U** – eigenvectors
- **stds** – geodesic directions

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 15-Mar-2018

calc_fpca (*no=3, id=None*)

This function calculates vertical functional principal component analysis on aligned data

Parameters

- **no** (*int*) – number of components to extract (default = 3)
- **id** (*int*) – point to use for $f(0)$ (default = midpoint)

Return type fdavpca object containing

Return q_pca srsf principal directions

Return f_pca functional principal directions

Return latent latent values

Return coef coefficients

Return U eigenvectors

plot ()

plot plot elastic vertical fPCA result Usage: obj.plot()

ELASTIC FUNCTIONAL BOXPLOTS

Elastic Functional Boxplots

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

class boxplots.**ampbox** (*fdawarp*)

This class provides amplitude boxplot for functional data using the SRVF framework

Usage: obj = ampbox(warp_data)

Parameters

- **warp_data** (*fdawarp*) – fdawarp class with alignment data
- **Q1** – First quartile
- **Q3** – Second quartile
- **Q1a** – First quantile based on alpha
- **Q3a** – Second quantile based on alpha
- **minn** – minimum extreme function
- **maxx** – maximum extreme function
- **outlier_index** – indexes of outlier functions
- **f_median** – median function
- **q_median** – median srvf
- **plt** – surface plot mesh

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 15-Mar-2018

construct_boxplot (*alpha=0.05, k_a=1*)

This function constructs the amplitude boxplot using the elastic square-root slope (srsf) framework.

Parameters

- **alpha** – quantile value (e.g.,=.05, i.e., 95%)
- **k_a** – scalar for outlier cutoff (e.g.,=1)

Return type ampbox object containing

Return warp_data aligned functions - fdawarp object

Return Q1 First quartile

Return Q3 Second quartile

Return Q1a First quantile based on alpha

Return Q3a Second quantile based on alpha

Return minn minimum extreme function

Return maxx maximum extreme function

Return outlier_index indexes of outlier functions

Return f_median median function

Return q_median median srsf

Return plt surface plot mesh

class `boxplots.phbox` (*fdawarp*)

This class provides phase boxplot for functional data using the SRVF framework

Usage: `obj = phbox(warp_data)`

Parameters

- **warp_data** (*fdawarp*) – fdawarp class with alignment data
- **Q1** – First quartile
- **Q3** – Second quartile
- **Q1a** – First quantile based on alpha
- **Q3a** – Second quantile based on alpha
- **minn** – minimum extreme function
- **maxx** – maximum extreme function
- **outlier_index** – indexes of outlier functions
- **median_x** – median warping function
- **psi_median** – median srvf of warping function
- **plt** – surface plot mesh

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 15-Mar-2018

construct_boxplot (*alpha=0.05, k_a=1*)

This function constructs phase boxplot for functional data using the elastic square-root slope (srsf) framework.

Parameters

- **alpha** – quantile value (e.g.,=.05, i.e., 95%)
- **k_a** – scalar for outlier cutoff (e.g.,=1)

Return type phbox object containing

Return warp_data fdawarp object

Return Q1 First quartile

Return Q3 Second quartile

Return Q1a First quantile based on alpha

Return Q3a Second quantile based on alpha

Return minn minimum extreme function

Return maxx maximum extreme function

Return outlier_index indexes of outlier functions

Return median_x median warping function

Return psi_median median srsf of warping function

Return plt surface plot mesh

plot()

plot box plot and surface plot

Usage: obj.plot()

FUNCTIONAL PRINCIPAL LEAST SQUARES

Partial Least Squares using SVD

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

fPLS **.pls_svd** (*time, qf, qg, no, alpha=0.0*)

This function computes the partial least squares using SVD

Parameters

- **time** – vector describing time samples
- **qf** – numpy ndarray of shape (M,N) of N functions with M samples
- **qg** – numpy ndarray of shape (M,N) of N functions with M samples
- **no** – number of components
- **alpha** – amount of smoothing (Default = 0.0 i.e., none)

Return type numpy ndarray

Return wqf f weight function

Return wqg g weight function

Return alpha smoothing value

Return values singular values

ELASTIC REGRESSION

Warping Invariant Regression using SRSF

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`regression.elastic_logistic(f, y, time, B=None, df=20, max_itr=20, cores=-1, smooth=False)`

This function identifies a logistic regression model with phase-variability using elastic methods

Parameters

- **f** (`np.ndarray`) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of labels (1/-1)
- **time** (`np.ndarray`) – vector of size M describing the sample points
- **B** – optional matrix describing Basis elements
- **df** – number of degrees of freedom B-spline (default 20)
- **max_itr** – maximum number of iterations (default 20)
- **cores** – number of cores for parallel processing (default all)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

Return fn aligned functions - numpy ndarray of shape (M,N) of M

functions with N samples :return qn: aligned srvfs - similar structure to fn :return gamma: calculated warping functions :return q: original training SRSFs :return B: basis matrix :return b: basis coefficients :return Loss: logistic loss

`regression.elastic_mlogistic(f, y, time, B=None, df=20, max_itr=20, cores=-1, delta=0.01, parallel=True, smooth=False)`

This function identifies a multinomial logistic regression model with phase-variability using elastic methods

Parameters

- **f** (`np.ndarray`) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of labels {1,2,...,m} for m classes
- **time** (`np.ndarray`) – vector of size M describing the sample points
- **B** – optional matrix describing Basis elements
- **df** – number of degrees of freedom B-spline (default 20)
- **max_itr** – maximum number of iterations (default 20)

- **cores** – number of cores for parallel processing (default all)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

Return fn aligned functions - numpy ndarray of shape (M,N) of N

functions with M samples :return qn: aligned srvfs - similar structure to fn :return gamma: calculated warping functions :return q: original training SRSFs :return B: basis matrix :return b: basis coefficients :return Loss: logistic loss

`regression.elastic_prediction(f, time, model, y=None, smooth=False)`

This function performs prediction from an elastic regression model with phase-variability

Parameters

- **f** – numpy ndarray of shape (M,N) of N functions with M samples
- **time** – vector of size M describing the sample points
- **model** – identified model from elastic_regression
- **y** – truth, optional used to calculate SSE

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

Return fn aligned functions - numpy ndarray of shape (M,N) of N

functions with M samples :return qn: aligned srvfs - similar structure to fn :return gamma: calculated warping functions :return q: original training SRSFs :return B: basis matrix :return b: basis coefficients :return SSE: sum of squared error

`regression.elastic_regression(f, y, time, B=None, lam=0, df=20, max_itr=20, cores=-1, smooth=False)`

This function identifies a regression model with phase-variability using elastic methods

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of N responses
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **B** – optional matrix describing Basis elements
- **lam** – regularization parameter (default 0)
- **df** – number of degrees of freedom B-spline (default 20)
- **max_itr** – maximum number of iterations (default 20)
- **cores** – number of cores for parallel processing (default all)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

Return fn aligned functions - numpy ndarray of shape (M,N) of M

functions with N samples :return qn: aligned srvfs - similar structure to fn :return gamma: calculated warping functions :return q: original training SRSFs :return B: basis matrix :return b: basis coefficients :return SSE: sum of squared error

`regression.logistic_warp(beta, time, q, y)`
calculates optimal warping for function logistic regression

Parameters

- **beta** – numpy ndarray of shape (M,N) of N functions with M samples
- **time** – vector of size N describing the sample points
- **q** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses

Return type numpy array

Return gamma warping function

`regression.logit_gradient(b, X, y)`
calculates gradient of the logistic loss

Parameters

- **b** – numpy ndarray of shape (M,N) of N functions with M samples
- **X** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses

Return type numpy array

Return grad gradient of logisitic loss

`regression.logit_hessian(s, b, X, y)`
calculates hessian of the logistic loss

Parameters

- **s** – numpy ndarray of shape (M,N) of N functions with M samples
- **b** – numpy ndarray of shape (M,N) of N functions with M samples
- **X** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses

Return type numpy array

Return out hessian of logistic loss

`regression.logit_loss(b, X, y)`
logistic loss function, returns $\text{Sum}\{-\log(\phi(t))\}$

Parameters

- **b** – numpy ndarray of shape (M,N) of N functions with M samples
- **X** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) of N responses

Return type numpy array

Return out loss value

`regression.mlogit_gradient(b, X, Y)`
calculates gradient of the multinomial logistic loss

Parameters

- **b** – numpy ndarray of shape (M,N) of N functions with M samples
- **x** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses

Return type numpy array

Return grad gradient

`regression.mlogit_loss(b, X, Y)`
calculates multinomial logistic loss (negative log-likelihood)

Parameters

- **b** – numpy ndarray of shape (M,N) of N functions with M samples
- **x** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses

Return type numpy array

Return nll negative log-likelihood

`regression.mlogit_warp_grad(alpha, beta, time, q, y, max_itr=8000, tol=1e-10, delta=0.008, display=0)`
calculates optimal warping for functional multinomial logistic regression

Parameters

- **alpha** – scalar
- **beta** – numpy ndarray of shape (M,N) of N functions with M samples
- **time** – vector of size M describing the sample points
- **q** – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy ndarray of shape (1,N) responses
- **max_itr** – maximum number of iterations (Default=8000)
- **tol** – stopping tolerance (Default=1e-10)
- **delta** – gradient step size (Default=0.008)
- **display** – display iterations (Default=0)

Return type tuple of numpy array

Return gam_old warping function

`regression.phi(t)`
calculates logistic function, returns $1 / (1 + \exp(-t))$

Parameters **t** – scalar

Return type numpy array

Return out return value

`regression.regression_warp(beta, time, q, y, alpha)`
calculates optimal warping for function linear regression

Parameters

- **beta** – numpy ndarray of shape (M,N) of M functions with N samples
- **time** – vector of size N describing the sample points
- **q** – numpy ndarray of shape (M,N) of M functions with N samples
- **y** – numpy ndarray of shape (1,N) of M functions with N samples

responses :param alpha: numpy scalar

Return type numpy array

Return gamma_new warping function

ELASTIC PRINCIPAL COMPONENT REGRESSION

Warping PCR Invariant Regression using SRSF

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

```
pcr_regression.elastic_lpcr_regression(f, y, time, pca_method='combined', no=5,  
                                     smooth_data=False, sparam=25)
```

This function identifies a logistic regression model with phase-variability using elastic pca

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of N responses
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **pca_method** – string specifying pca method (options = “combined”, “vert”, or “horiz”, default = “combined”)
- **no** – scalar specify number of principal components (default=5)
- **smooth_data** – smooth data using box filter (default = F)
- **sparam** – number of times to apply box filter (default = 25)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return b regressor vector

Return y response vector

Return warp_data alignment object from srsf_align

Return pca fpca object from corresponding pca method

Return Loss logistic loss

Return pca.method string of pca method

```
pcr_regression.elastic_mlpcr_regression(f, y, time, pca_method='combined', no=5,  
                                       smooth_data=False, sparam=25)
```

This function identifies a logistic regression model with phase-variability using elastic pca

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of N responses
- **time** (*np.ndarray*) – vector of size M describing the sample points

- **pca_method** – string specifying pca method (options = “combined”, “vert”, or “horiz”, default = “combined”)
- **no** – scalar specify number of principal components (default=5)
- **smooth_data** – smooth data using box filter (default = F)
- **sparam** – number of times to apply box filter (default = 25)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return b regressor vector

Return y response vector

Return warp_data alignment object from srsf_align

Return pca fpca object from corresponding pca method

Return Loss logistic loss

Return pca.method string of pca method

```

pcr_regression.elastic_pcr_regression(f, y, time, pca_method='combined', no=5,
                                     smooth_data=False, sparam=25, parallel=False,
                                     C=None)

```

This function identifies a regression model with phase-variability using elastic pca

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **y** – numpy array of N responses
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **pca_method** – string specifying pca method (options = “combined”, “vert”, or “horiz”, default = “combined”)
- **no** – scalar specify number of principal components (default=5)
- **smooth_data** – smooth data using box filter (default = F)
- **sparam** – number of times to apply box filter (default = 25)
- **parallel** – run in parallel (default = F)
- **C** – scale balance parameter for combined method (default = None)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return b regressor vector

Return y response vector

Return warp_data alignment object from srsf_align

Return pca fpca object from corresponding pca method

Return SSE sum of squared errors

Return pca.method string of pca method

ELASTIC FUNCTIONAL TOLERANCE BOUNDS

Functional Tolerance Bounds using SRSF

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`tolerance.bootTB` (*f*, *time*, *a*=0.5, *p*=0.99, *B*=500, *no*=5, *parallel*=True)

This function computes tolerance bounds for functional data containing phase and amplitude variation using bootstrap sampling

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **a** – confidence level of tolerance bound (default = 0.05)
- **p** – coverage level of tolerance bound (default = 0.99)
- **B** – number of bootstrap samples (default = 500)
- **no** – number of principal components (default = 5)
- **parallel** – enable parallel processing (default = T)

Return type tuple of boxplot objects

Return amp amplitude tolerance bounds

Rtype out_med ampbox object

Return ph phase tolerance bounds

Rtype out_med phbox object

Return out_med alignment results

Rtype out_med fdawarp object

`tolerance.mvtol_region` (*x*, *alpha*, *P*, *B*)

Computes tolerance factor for multivariate normal

Krishnamoorthy, K. and Mondal, S. (2006), Improved Tolerance Factors for Multivariate Normal Distributions, Communications in Statistics - Simulation and Computation, 35, 461–478.

Parameters

- **x** – (M,N) matrix defining N variables of M samples
- **alpha** – confidence level
- **P** – coverage level
- **B** – number of bootstrap samples

Return type double

Return tol tolerance factor

`tolerance.pcaTB(f, time, a=0.5, p=0.99, no=5, parallel=True)`

This function computes tolerance bounds for functional data containing phase and amplitude variation using fPCA

Parameters

- **f** (*np.ndarray*) – numpy ndarray of shape (M,N) of N functions with M samples
- **time** (*np.ndarray*) – vector of size M describing the sample points
- **a** – confidence level of tolerance bound (default = 0.05)
- **p** – coverage level of tolerance bound (default = 0.99)
- **no** – number of principal components (default = 5)
- **parallel** – enable parallel processing (default = T)

Return type tuple of boxplot objects

Return warp alignment data from time_warping

Return pca functional pca from jointFPCA

Return tol tolerance factor

`tolerance.rwishart(df, p)`

Computes a random wishart matrix

Parameters

- **df** – degree of freedom
- **p** – number of dimensions

Return type double

Return R matrix

SRVF GEODESIC COMPUTATION

geodesic calculation for SRVF (curves) open and closed)

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`geodesic.back_parallel_transport` (*u1*, *alpha*, *basis*, *T=100*, *k=5*)
backwards parallel translates q1 and q2 along manifold

Parameters

- **u1** – numpy ndarray of shape (2,M) of M samples
- **alpha** – numpy ndarray of shape (2,M) of M samples
- **basis** – list numpy ndarray of shape (2,M) of M samples
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return utilde translated vector

`geodesic.calc_alphadot` (*alpha*, *basis*, *T=100*, *k=5*)
calculates derivative along the path alpha

Parameters

- **alpha** – numpy ndarray of shape (2,M) of M samples
- **basis** – list of numpy ndarray of shape (2,M) of M samples
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return alphadot derivative of alpha

`geodesic.calculate_energy` (*alphadot*, *T=100*, *k=5*)
calculates energy along path

Parameters

- **alphadot** – numpy ndarray of shape (2,M) of M samples
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy scalar

Return E energy

`geodesic.calculate_gradE(u, utilde, T=100, k=5)`
calculates gradient of energy along path

Parameters

- **u** – numpy ndarray of shape (2,M) of M samples
- **utilde** – numpy ndarray of shape (2,M) of M samples
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy scalar

Return gradE gradient of energy

Return normgradE norm of gradient of energy

`geodesic.cov_integral(alpha, alphadot, basis, T=100, k=5)`
Calculates covariance along path alpha

Parameters

- **alpha** – numpy ndarray of shape (2,M) of M samples (first curve)
- **alphadot** – numpy ndarray of shape (2,M) of M samples
- **basis** – list numpy ndarray of shape (2,M) of M samples
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return u covariance

`geodesic.find_basis_normal_path(alpha, k=5)`
computes orthonormalized basis vectors to the normal space at each of the k points (q-functions) of the path alpha

Parameters

- **alpha** – numpy ndarray of shape (2,M) of M samples (path)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return basis basis vectors along the path

`geodesic.geod_dist_path_strt(beta, k=5)`
calculate geodesic distance for path straightening

Parameters

- **beta** – numpy ndarray of shape (2,M) of M samples
- **k** – number of samples along path (Default = 5)

Return type numpy scalar

Return dist geodesic distance

`geodesic.geod_sphere(beta1, beta2, k=5)`
This function calculates the geodesic between open curves beta1 and beta2 with k steps along path

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples
- **beta2** – numpy ndarray of shape (2,M) of M samples
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return dist geodesic distance

Return path geodesic path

Return O rotation matrix

`geodesic.init_path_geod(beta1, beta2, T=100, k=5)`

Initializes a path in $\text{cal}\{C\}$. beta1, beta2 are already standardized curves. Creates a path from beta1 to beta2 in shape space, then projects to the closed shape manifold.

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples (first curve)
- **beta2** – numpy ndarray of shape (2,M) of M samples (end curve)
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return alpha a path between two q-functions

Return beta a path between two curves

Return O rotation matrix

`geodesic.init_path_rand(beta1, beta_mid, beta2, T=100, k=5)`

Initializes a path in $\text{cal}\{C\}$. beta1, beta_mid, beta2 are already standardized curves. Creates a path from beta1 to beta_mid to beta2 in shape space, then projects to the closed shape manifold.

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples (first curve)
- **betamid** – numpy ndarray of shape (2,M) of M samples (mid curve)
- **beta2** – numpy ndarray of shape (2,M) of M samples (end curve)
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return alpha a path between two q-functions

Return beta a path between two curves

Return O rotation matrix

`geodesic.path_straightening(beta1, beta2, betamid, init='rand', T=100, k=5)`

Perform path straightening to find geodesic between two shapes in either the space of closed curves or the space of affine standardized curves. This algorithm follows the steps outlined in section 4.6 of the manuscript.

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples (first curve)

- **beta2** – numpy ndarray of shape (2,M) of M samples (end curve)
- **betamid** – numpy ndarray of shape (2,M) of M samples (mid curve Default = NULL, only needed for init “rand”)
- **init** – initialize path geodesic or random (Default = “rand”)
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy ndarray

Return dist geodesic distance

Return path geodesic path

Return pathsqnc geodesic path sequence

Return E energy

`geodesic.update_path(alpha, beta, gradE, delta, T=100, k=5)`

Update the path along the direction -gradE

Parameters

- **alpha** – numpy ndarray of shape (2,M) of M samples
- **beta** – numpy ndarray of shape (2,M) of M samples
- **gradE** – numpy ndarray of shape (2,M) of M samples
- **delta** – gradient parameter
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

Return type numpy scalar

Return alpha updated path of srvfs

Return beta updated path of curves

UTILITY FUNCTIONS

Utility functions for SRSF Manipulations

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`utility_functions.SqrtMean(gam)`

calculates the srsf of warping functions with corresponding shooting vectors

Parameters **gam** – numpy ndarray of shape (M,N) of M warping functions with N samples

Return type 2 numpy ndarray and vector

Return mu Karcher mean psi function

Return gam_mu vector of dim N which is the Karcher mean warping function

Return psi numpy ndarray of shape (M,N) of M SRSF of the warping functions

Return vec numpy ndarray of shape (M,N) of M shooting vectors

`utility_functions.SqrtMeanInverse(gam)`

finds the inverse of the mean of the set of the diffeomorphisms gamma

Parameters **gam** – numpy ndarray of shape (M,N) of M warping functions with N samples

Return type vector

Return gamI inverse of gam

`utility_functions.SqrtMedian(gam)`

calculates the median srsf of warping functions with corresponding shooting vectors

Parameters **gam** – numpy ndarray of shape (M,N) of M warping functions with N samples

Return type 2 numpy ndarray and vector

Return gam_median Karcher median warping function

Return psi_meidan vector of dim N which is the Karcher median srsf function

Return psi numpy ndarray of shape (M,N) of M SRSF of the warping functions

Return vec numpy ndarray of shape (M,N) of M shooting vectors

`utility_functions.cumtrapzmid(x, y, c, mid)`

cumulative trapezoidal numerical integration taken from midpoint

Parameters

- **x** – vector of size N describing the time samples
- **y** – vector of size N describing the function
- **c** – midpoint

- **mid** – midpiont location

Return type vector

Return fa cumulative integration

`utility_functions.diffop(n, binsize=1)`

Creates a second order differential operator

Parameters

- **n** – dimension
- **binsize** – dx (default = 1)

Return type numpy ndarray

Return m matrix describing differential operator

`utility_functions.elastic_distance(f1, f2, time, lam=0.0)`

” calculates the distances between function, where f1 is aligned to f2. In other words calculates the elastic distances

Parameters

- **f1** – vector of size N
- **f2** – vector of size N
- **time** – vector of size N describing the sample points
- **lam** – controls the elasticity (default = 0.0)

Return type scalar

Return Dy amplitude distance

Return Dx phase distance

`utility_functions.f_K_fold(Nobs, K=5)`

generates sample indices for K-fold cross validation

:param Nobs number of observations :param K number of folds

Return type numpy ndarray

Return train train indexes (Nobs*(K-1)/K X K)

Return test test indexes (Nobs*(1/K) X K)

`utility_functions.f_to_srsf(f, time, smooth=False)`

converts f to a square-root slope function (SRSF)

Parameters

- **f** – vector of size N samples
- **time** – vector of size N describing the sample points

Return type vector

Return q srsf of f

`utility_functions.geigen(Amat, Bmat, Cmat)`

generalized eigenvalue problem of the form

$\max \text{tr } L'AM / \sqrt{\text{tr } L'BL \text{tr } M'CM}$ w.r.t. L and M

:param Amat numpy ndarray of shape (M,N) :param Bmat numpy ndarray of shape (M,N) :param Bmat numpy ndarray of shape (M,N)

Return type numpy ndarray

Return values eigenvalues

Return Lmat left eigenvectors

Return Mmat right eigenvectors

`utility_functions.gradient_spline(time, f, smooth=False)`

This function takes the gradient of f using b-spline smoothing

Parameters

- **time** – vector of size N describing the sample points
- **f** – numpy ndarray of shape (M,N) of M functions with N samples
- **smooth** – smooth data (default = F)

Return type tuple of numpy ndarray

Return f0 smoothed functions functions

Return g first derivative of each function

Return g2 second derivative of each function

`utility_functions.innerprod_q(time, q1, q2)`

calculates the innerproduct between two srsfs

:param time vector describing time samples :param q1 vector of srsf 1 :param q2 vector of srsf 2

Return type scalar

Return val inner product value

`utility_functions.invertGamma(gam)`

finds the inverse of the diffeomorphism gamma

Parameters **gam** – vector describing the warping function

Return type vector

Return gamI inverse of gam

`utility_functions.optimum_reparam(q1, time, q2, method='DP', lam=0.0, flo=0.0, f2o=0.0)`

calculates the warping to align srsf q2 to q1

Parameters

- **q1** – vector of size N or array of NxM samples of first SRSF
- **time** – vector of size N describing the sample points
- **q2** – vector of size N or array of NxM samples of second SRSF
- **method** – method to apply optimization (default="DP") options are "DP", "DP2" and "RBFSGS"
- **lam** – controls the amount of elasticity (default = 0.0)

Return type vector

Return gam describing the warping function used to align q2 with q1

`utility_functions.optimum_reparam_pair(q, time, q1, q2, lam=0.0)`
calculates the warping to align srsf pair q1 and q2 to q

Parameters

- **q** – vector of size N or array of NxM samples of first SRSF
- **time** – vector of size N describing the sample points
- **q1** – vector of size N or array of NxM samples of second SRSF
- **q2** – vector of size N or array of NxM samples of second SRSF
- **lam** – controls the amount of elasticity (default = 0.0)

Return type vector

Return gam describing the warping function used to align q2 with q1

`utility_functions.outlier_detection(q, time, mq, k=1.5)`
calculates outlier's using geodesic distances of the SRSFs from the median

Parameters

- **q** – numpy ndarray of N x M of M SRS functions with N samples
- **time** – vector of size N describing the sample points
- **mq** – median calculated using `time_warping.srsf_align()`
- **k** – cutoff threshold (default = 1.5)

Returns q_outlier: outlier functions

`utility_functions.randomGamma(gam, num)`
generates random warping functions

Parameters

- **gam** – numpy ndarray of N x M of M of warping functions
- **num** – number of random functions

Returns rgam: random warping functions

`utility_functions.resamplefunction(x, n)`
resample function using n points

Parameters

- **x** – functions
- **n** – number of points

Return type numpy array

Return xn resampled function

`utility_functions.rgam(N, sigma, num)`
Generates random warping functions

Parameters

- **N** – length of warping function
- **sigma** – variance of warping functions
- **num** – number of warping functions

Returns gam: numpy ndarray of warping functions

`utility_functions.smooth_data(f, sparam)`

This function smooths a collection of functions using a box filter

Parameters

- **f** – numpy ndarray of shape (M,N) of M functions with N samples
- **sparam** – Number of times to run box filter (default = 25)

Return type numpy ndarray

Return f smoothed functions

`utility_functions.srsf_to_f(q, time, f0=0.0)`

converts q (srsf) to a function

Parameters

- **q** – vector of size N samples of srsf
- **time** – vector of size N describing time sample points
- **f0** – initial value

Return type vector

Return f function

`utility_functions.update_progress(progress)`

This function creates a progress bar

Parameters **progress** – fraction of progress

`utility_functions.warp_f_gamma(time, f, gam)`

warps a function f by gam

:param time vector describing time samples :param q vector describing srsf :param gam vector describing warping function

Return type numpy ndarray

Return f_temp warped srsf

`utility_functions.warp_q_gamma(time, q, gam)`

warps a srsf q by gam

:param time vector describing time samples :param q vector describing srsf :param gam vector describing warping function

Return type numpy ndarray

Return q_temp warped srsf

`utility_functions.zero_crossing(Y, q, bt, time, y_max, y_min, gmax, gmin)`

finds zero-crossing of optimal gamma, $\text{gam} = s \cdot \text{gmax} + (1-s) \cdot \text{gmin}$ from elastic regression model

Parameters

- **Y** – response
- **q** – predictive function
- **bt** – basis function
- **time** – time samples
- **y_max** – maximum response for warping function gmax
- **y_min** – minimum response for warping function gmin

- **gmax** – max warping function
- **gmin** – min warping fuction

Return type numpy array

Return gamma optimal warping function

CURVE FUNCTIONS

functions for SRVF curve manipulations

moduleauthor:: Derek Tucker <jdtuck@sandia.gov>

`curve_functions.calc_j(basis)`

Calculates Jacobian matrix from normal basis

Parameters **basis** – list of numpy ndarray of shape (2,M) of M samples basis

Return type numpy ndarray

Return j Jacobian

`curve_functions.calculate_variance(beta)`

This function calculates variance of curve beta

Parameters **beta** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return variance variance

`curve_functions.calculatecentroid(beta)`

This function calculates centroid of a parameterized curve

Parameters **beta** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return centroid center coordinates

`curve_functions.curve_to_q(beta)`

This function converts curve beta to srvf q

Parameters **beta** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return q srvf of curve

`curve_functions.curve_zero_crossing(Y, beta, bt, y_max, y_min, gmax, gmin)`

finds zero-crossing of optimal gamma, $\text{gam} = s * g_{\text{max}} + (1-s) * g_{\text{min}}$ from elastic curve regression model

Parameters

- **Y** – response
- **beta** – predictive function
- **bt** – basis function
- **y_max** – maximum response for warping function gmax

- **y_min** – minimum response for warping function gmin
- **gmax** – max warping function
- **gmin** – min warping function

Return type numpy array

Return gamma optimal warping function

Return O_hat rotation matrix

`curve_functions.find_basis_normal(q)`

Finds the basis normal to the srvf

Parameters **q1** – numpy ndarray of shape (2,M) of M samples

Return type list of numpy ndarray

Return basis list containing basis vectors

`curve_functions.find_best_rotation(q1, q2)`

This function calculates the best rotation between two srvfs using procustes rigid alignment

Parameters

- **q1** – numpy ndarray of shape (2,M) of M samples
- **q2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return q2new optimal rotated q2 to q1

Return R rotation matrix

`curve_functions.find_rotation_and_seed_coord(beta1, beta2)`

This function returns a candidate list of optimally oriented and registered (seed) shapes w.r.t. beta1

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples
- **beta2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return beta2new optimal rotated beta2 to beta1

Return O rotation matrix

Return tau seed

`curve_functions.find_rotation_and_seed_q(q1, q2)`

This function returns a candidate list of optimally oriented and registered (seed) shapes w.r.t. beta1

Parameters

- **q1** – numpy ndarray of shape (2,M) of M samples
- **q2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return beta2new optimal rotated beta2 to beta1

Return O rotation matrix

Return tau seed

`curve_functions.gram_schmidt` (*basis*)

Performs Gram Schmidt Orthogonalization of a basis_o

param basis list of numpy ndarray of shape (2,M) of M samples

rtype list of numpy ndarray

return basis_o orthogonalized basis

`curve_functions.group_action_by_gamma` (*q, gamma*)

This function reparameterized srvf q by gamma

Parameters

- **f** – numpy ndarray of shape (2,M) of M samples
- **gamma** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return qn reparameterized srvf

`curve_functions.group_action_by_gamma_coord` (*f, gamma*)

This function reparameterized curve f by gamma

Parameters

- **f** – numpy ndarray of shape (2,M) of M samples
- **gamma** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return fn reparameterized curve

`curve_functions.innerprod_q2` (*q1, q2*)

This function calculates the inner product in srvf space

Parameters

- **q1** – numpy ndarray of shape (2,M) of M samples
- **q2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return val inner product

`curve_functions.inverse_exp` (*q1, q2, beta2*)

Calculate the inverse exponential to obtain a shooting vector from q1 to q2 in shape space of open curves

Parameters

- **q1** – numpy ndarray of shape (2,M) of M samples
- **q2** – numpy ndarray of shape (2,M) of M samples
- **beta2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return v shooting vectors

`curve_functions.inverse_exp_coord` (*beta1, beta2*)

Calculate the inverse exponential to obtain a shooting vector from beta1 to beta2 in shape space of open curves

Parameters

- **beta1** – numpy ndarray of shape (2,M) of M samples

- **beta2** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return v shooting vectors

Return dist distance

`curve_functions.optimum_reparam_curve(q1, q2, lam=0.0)`
calculates the warping to align srsf q2 to q1

Parameters

- **q1** – matrix of size nxN or array of NxM samples of first SRVF
- **time** – vector of size N describing the sample points
- **q2** – matrix of size nxN or array of NxM samples of second SRVF
- **lam** – controls the amount of elasticity (default = 0.0)

Return type vector

Return gam describing the warping function used to align q2 with q1

`curve_functions.parallel_translate(w, q1, q2, basis, mode=0)`
parallel translates q1 and q2 along manifold

Parameters

- **w** – numpy ndarray of shape (2,M) of M samples
- **q1** – numpy ndarray of shape (2,M) of M samples
- **q2** – numpy ndarray of shape (2,M) of M samples
- **basis** – list of numpy ndarray of shape (2,M) of M samples
- **mode** – open 0 or closed curves 1 (default 0)

Return type numpy ndarray

Return wbar translated vector

`curve_functions.pre_proc_curve(beta, T=100)`
This function preprocessed a curve beta to set of closed curves

Parameters

- **beta** – numpy ndarray of shape (2,M) of M samples
- **T** – number of samples (default = 100)

Return type numpy ndarray

Return betanew projected beta

Return qnew projected srvf

Return A alignment matrix (not used currently)

`curve_functions.project_curve(q)`
This function projects srvf q to set of close curves

Parameters **q** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return qproj project srvf

`curve_functions.project_tangent(w, q, basis)`

projects srvf to tangent space w using basis

Parameters

- **w** – numpy ndarray of shape (2,M) of M samples
- **q** – numpy ndarray of shape (2,M) of M samples
- **basis** – list of numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return wproj projected q

`curve_functions.psi(x, a, q)`

This function formats variance output

Parameters

- **x** – numpy ndarray of shape (2,M) of M samples curve
- **a** – numpy ndarray of shape (2,1) mean
- **q** – numpy ndarray of shape (2,M) of M samples srvf

Return type numpy ndarray

Return psi1 variance

Return psi2 cross variance

Return psi3 curve end

Return psi4 curve end

`curve_functions.q_to_curve(q)`

This function converts srvf to beta

Parameters **q** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return beta parameterized curve

`curve_functions.resamplecurve(x, N=100)`

This function resamples a curve to have N samples

Parameters

- **x** – numpy ndarray of shape (2,M) of M samples
- **N** – Number of samples for new curve (default = 100)

Return type numpy ndarray

Return xn resampled curve

`curve_functions.scale_curve(beta)`

scales curve to length 1

Parameters **beta** – numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return beta_scaled scaled curve

Return scale scale factor used

`curve_functions.shift_f(f, tau)`
shifts a curve f by τ

Parameters

- **f** – numpy ndarray of shape (2,M) of M samples
- **tau** – scalar

Return type numpy ndarray

Return fn shifted curve

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