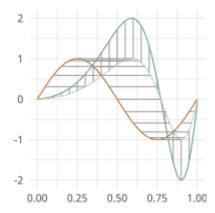
fdasrsf Documentation

Release 2.3.8

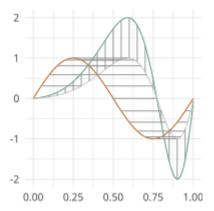
J. Derek Tucker

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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.



CONTENTS 1

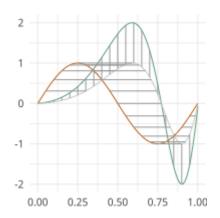
2 CONTENTS

CHAPTER

ONE

USER GUIDE

Contents:



1.1 Elastic Functional Alignment

Otherwise known as time warping in the literature is at the center of elastic functional data analysis. Here our goal is to separate out the horizontal and vertical variability of the functional data

```
[1]: import fdasrsf as fs import numpy as np
```

Load in our example data

```
[2]: data = np.load('../../bin/simu_data.npz')
  time = data['arr_1']
  f = data['arr_0']
```

We will then construct the fdawarp object

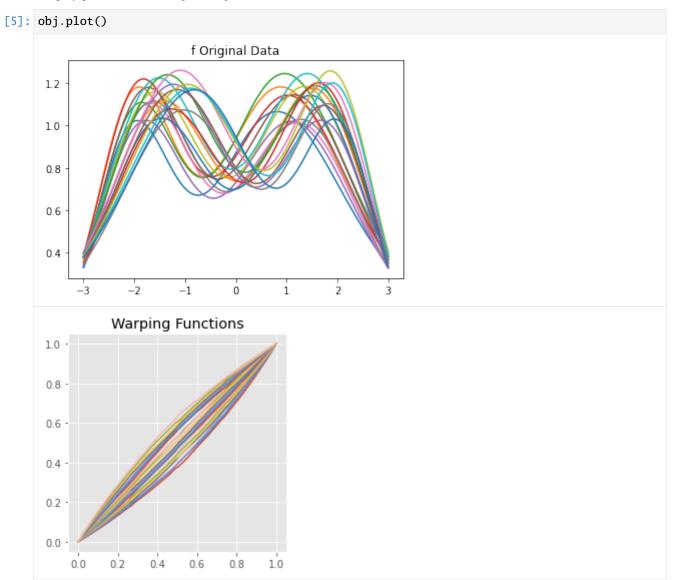
```
[3]: obj = fs.fdawarp(f,time)
```

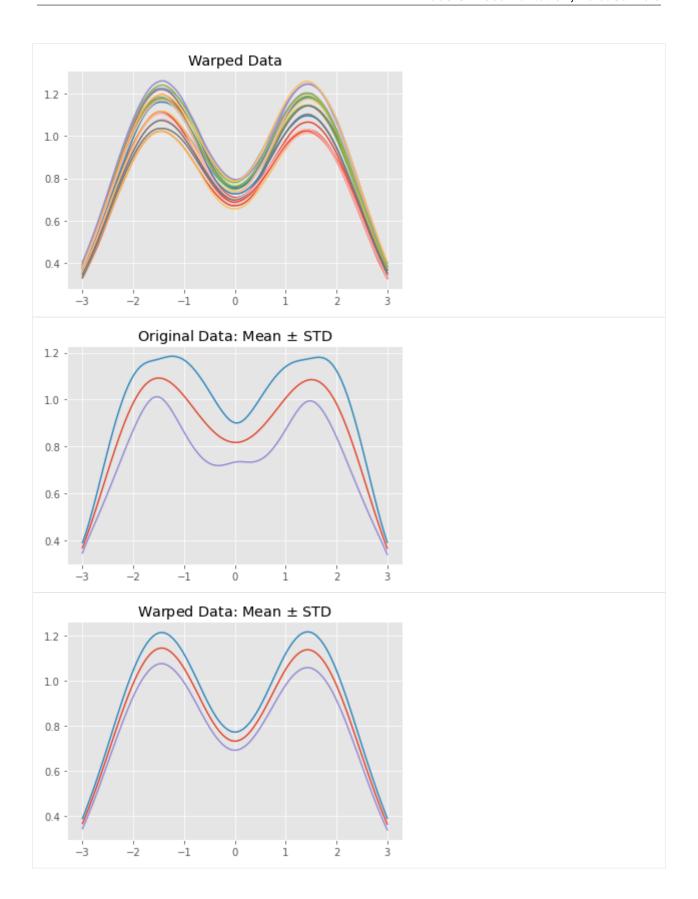
Next we will align the functions using the elastic framework

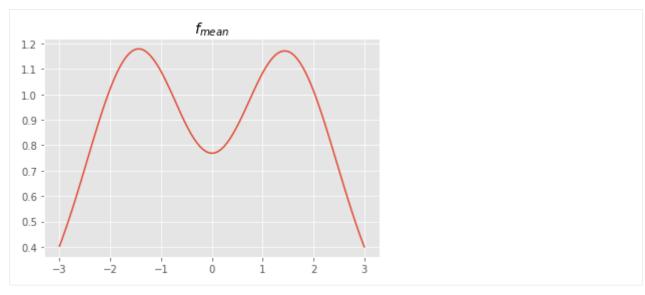
```
[4]: obj.srsf_align(parallel=True)

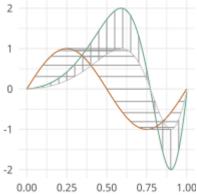
Initializing...
Compute Karcher Mean of 21 function in SRSF space...
updating step: r=1
updating step: r=2
```

Display plots demonstrating the alignment









1.2 Elastic Functional Principal Component Analysis

After we have aligned our data we can compute functional principal component analysis (fPCA) on the aligned data, warping functions, and jointly

```
[1]: import fdasrsf as fs import numpy as np
```

We will load in our example data again and compute the alignment

```
[2]: data = np.load('../../bin/simu_data.npz')
   time = data['arr_1']
   f = data['arr_0']
   obj = fs.fdawarp(f,time)
   obj.srsf_align(parallel=True)

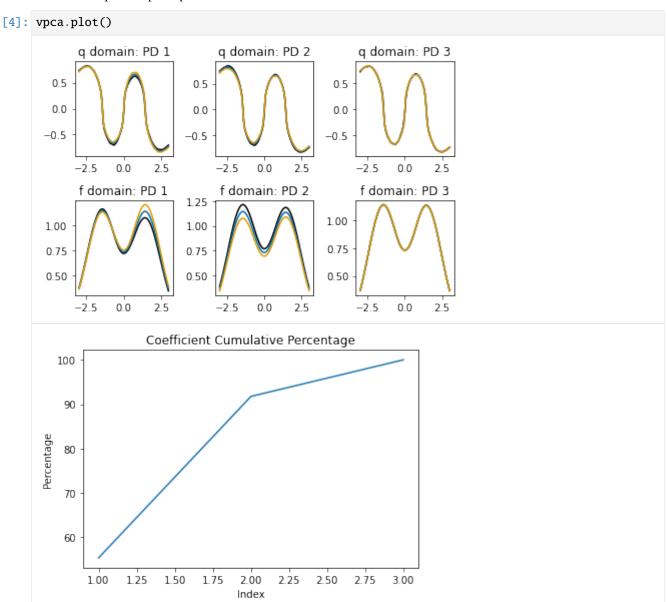
Initializing...
Compute Karcher Mean of 21 function in SRSF space...
   updating step: r=1
   updating step: r=2
```

1.2.1 Vertical fPCA

We will first compute fPCA on the aligned functions, by constructing the object and computing the PCA for the number of components, default=3)

[3]: vpca = fs.fdavpca(obj)
vpca.calc_fpca(no=3)

We then can plot the principal directions

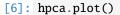


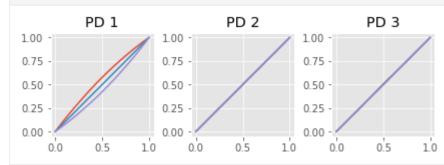
1.2.2 Horizontal fPCA

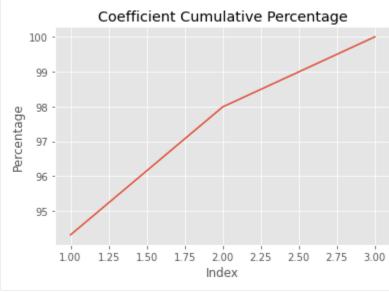
We can then compute PCA on the set of warping functions

[5]: hpca = fs.fdahpca(obj)
hpca.calc_fpca(no=3)

We then can plot the principal directions







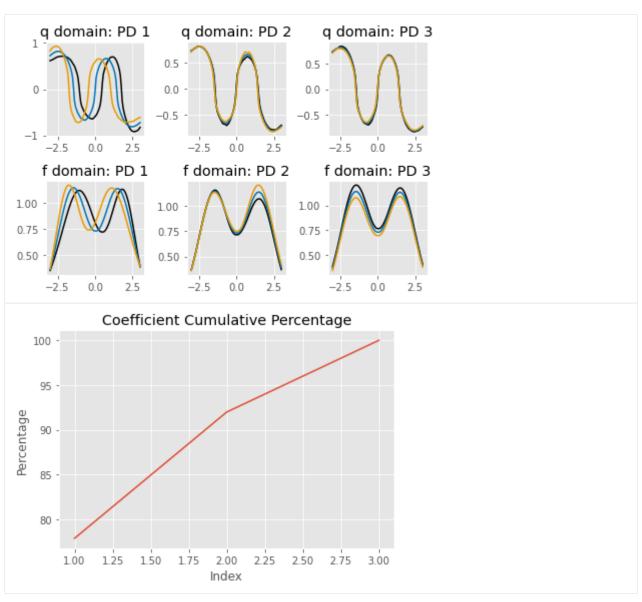
1.2.3 Joint fPCA

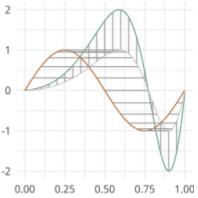
We can also compute the fPCA on jointly on the phase/amplitude space if we feel there is correlation between the variabilities

[7]: jpca = fs.fdajpca(obj)
 jpca.calc_fpca(no=3)

We then can plot the principal directions

[8]: jpca.plot()





1.3 Elastic Curve Alignment

Otherwise known as time warping in the literature is at the center of elastic functional data analysis. Here our goal is to separate out the horizontal and vertical variability of the open/closed curves

```
[1]: import fdasrsf as fs import numpy as np
```

Load in our example data

```
[2]: data = np.load('../../bin/MPEG7.npz',allow_pickle=True)
    Xdata = data['Xdata']
    curve = Xdata[0,1]
    n,M = curve.shape
    K = Xdata.shape[1]

beta = np.zeros((n,M,K))
    for i in range(0,K):
        beta[:,:,i] = Xdata[0,i]
```

We will then construct the fdacurve object

```
[3]: obj = fs.fdacurve(beta,N=M)
```

We then will compute karcher mean of the curves

```
[4]: obj.karcher_mean()

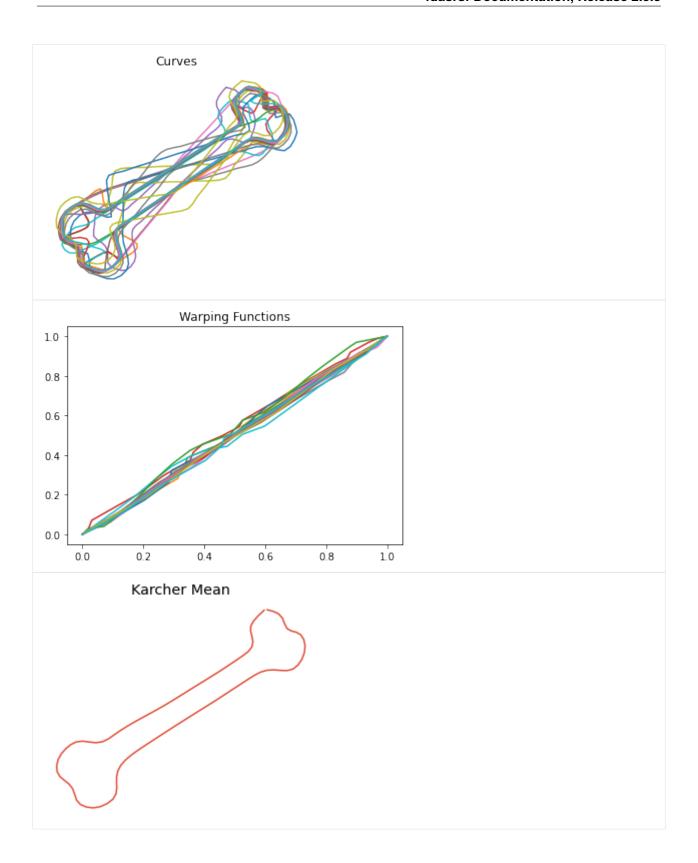
Computing Karcher Mean of 20 curves in SRVF space..
    updating step: 1
    updating step: 2
    updating step: 3
    updating step: 4
    updating step: 5
    updating step: 6
    updating step: 7
```

We then can align the curves to the karcher mean

```
[5]: obj.srvf_align(rotation=False)
```

Plot the results

```
[6]: obj.plot()
```

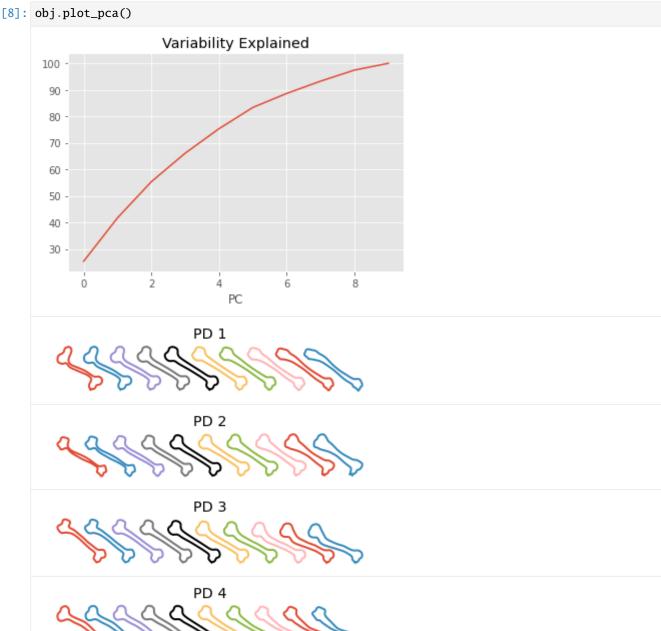


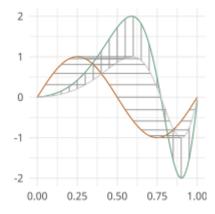
1.3.1 Shape PCA

We then can compute the Karcher covariance and compute the shape pca

[7]: obj.karcher_cov() obj.shape_pca()

Plot the principal directions





FUNCTIONAL ALIGNMENT

Group-wise function alignment using SRSF framework and Dynamic Programming

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

time_warping.align_fPCA(f, time, num_comp=3, showplot=True, smoothdata=False, cores=-1) 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)
- **cores** number of cores for parallel (default = -1 (all))

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 qg0: original srvf - similar structure to fn :return qg0: original srvf - similar structure to fn :return qg0: original srvf - similar structure to fn :return wqf: srsf principal weight functions :return wqg: 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

- $\mathbf{f} (M,N)$: 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 inverse 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)

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)

multiple_align_functions(mu, omethod='DP2', smoothdata=False, parallel=False, lam=0.0, cores=-1, grid dim=7)

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

Usage: obj.multiple_align_functions(mu) obj.multiple_align_functions(lambda)

obj.multiple_align_functions(lambda, ...)

Parameters

- mu vector of function to align to
- **omethod** optimization method (DP, DP2, RBFGS) (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)
- **cores** number of cores for parallel (default = -1 (all))
- **grid_dim** size of the grid, for the DP2 method only (default = 7)

plot()

plot plot functional alignment results

Usage: obj.plot()

srsf_align(method='mean', omethod='DP2', center=True, smoothdata=False, MaxItr=20, parallel=False,
lam=0.0, cores=-1, grid_dim=7)

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, RBFGS) (default = DP2)
- **center** center warping functions (default = T)
- **smoothdata** (bool) Smooth the data using a box filter (default = F)
- MaxItr Maximum number of iterations (default = 20)
- **parallel** run in parallel (default = F)
- lam (double) controls the elasticity (default = 0)
- cores number of cores for parallel (default = -1 (all))
- **grid_dim** size of the grid, for the DP2 method only (default = 7)

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()

time_warping.normal(loc=0.0, scale=1.0, size=None)

Draw random samples from a normal (Gaussian) distribution.

The probability density function of the normal distribution, first derived by De Moivre and 200 years later by both Gauss and Laplace independently², is often called the bell curve because of its characteristic shape (see the example below).

The normal distributions occurs often in nature. For example, it describes the commonly occurring distribution of samples influenced by a large number of tiny, random disturbances, each with its own unique distribution².

Note: New code should use the normal method of a default_rng() instance instead; please see the random-quick-start.

loc [float or array_like of floats] Mean ("centre") of the distribution.

scale [float or array_like of floats] Standard deviation (spread or "width") of the distribution. Must be non-negative.

size [int or tuple of ints, optional] Output shape. If the given shape is, e.g., (m, n, k), then m * n * k samples are drawn. If size is None (default), a single value is returned if loc and scale are both scalars. Otherwise, np.broadcast(loc, scale).size samples are drawn.

out [ndarray or scalar] Drawn samples from the parameterized normal distribution.

scipy.stats.norm [probability density function, distribution or] cumulative density function, etc.

Generator.normal: which should be used for new code.

The probability density for the Gaussian distribution is

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}},$$

where μ is the mean and σ the standard deviation. The square of the standard deviation, σ^2 , is called the variance.

The function has its peak at the mean, and its "spread" increases with the standard deviation (the function reaches 0.607 times its maximum at $x + \sigma$ and $x - \sigma^2$). This implies that normal is more likely to return samples lying close to the mean, rather than those far away.

Draw samples from the distribution:

² P. R. Peebles Jr., "Central Limit Theorem" in "Probability, Random Variables and Random Signal Principles", 4th ed., 2001, pp. 51, 51, 125.

```
>>> mu, sigma = 0, 0.1 # mean and standard deviation
>>> s = np.random.normal(mu, sigma, 1000)
```

Verify the mean and the variance:

```
>>> abs(mu - np.mean(s))
0.0 # may vary
```

```
>>> abs(sigma - np.std(s, ddof=1))
0.1 # may vary
```

Display the histogram of the samples, along with the probability density function:

Two-by-four array of samples from N(3, 6.25):

time_warping.pairwise_align_bayes(fli, f2i, time, mcmcopts=None)

This function aligns two functions using Bayesian framework. It will align f2 to f1. It is based on mapping warping functions to a hypersphere, and a subsequent exponential mapping to a tangent space. In the tangent space, the Z-mixture pCN algorithm is used to explore both local and global structure in the posterior distribution.

The Z-mixture pCN algorithm uses a mixture distribution for the proposal distribution, controlled by input parameter zpcn. The zpcn\$betas must be between 0 and 1, and are the coefficients of the mixture components, with larger coefficients corresponding to larger shifts in parameter space. The zpcn["probs"] give the probability of each shift size.

Usage: out = pairwise_align_bayes(f1i, f2i, time) out = pairwise_align_bayes(f1i, f2i, time, mcmcopts)

Parameters

- fli vector defining M samples of function 1
- **f2i** vector defining M samples of function 2
- time time vector of length M
- mcmopts dict of mcmc parameters

default mcmc options: tmp = {"betas":np.array([0.5,0.5,0.005,0.0001]),"probs":np.array([0.1,0.1,0.7,0.1])} mcmcopts = {"iter":2*(10**4), "burnin":np.minimum(5*(10**3),2*(10**4)//2),

```
"alpha0":0.1, "beta0":0.1,"zpcn":tmp,"propvar":1, "initcoef":np.repeat(0,20), "npoints":200, "extrainfo":True}
```

:rtype collection containing :return f2_warped: aligned f2 :return gamma: warping function :return g_coef: final g_coef :return psi: final psi :return sigma1: final sigma

if extrainfo :return accept: accept of psi samples :return betas_ind :return logl: log likelihood :return gamma_mat: posterior gammas :return gamma_stats: posterior gamma stats :return xdist: phase distance posterior :return ydist: amplitude distance posterior)

time_warping.pairwise_align_bayes_infHMC(y1i, y2i, time, mcmcopts=None)

This function aligns two functions using Bayesian framework. It uses a hierarchical Bayesian framework assuming mearsurement error error It will align f2 to f1. It is based on mapping warping functions to a hypersphere, and a subsequent exponential mapping to a tangent space. In the tangent space, the infty-HMC algorithm is used to explore both local and global structure in the posterior distribution.

Usage: out = pairwise_align_bayes_infHMC(f1i, f2i, time) out = pairwise_align_bayes_infHMC(f1i, f2i, time, mcmcopts)

Parameters

- y1i vector defining M samples of function 1
- y2i vector defining M samples of function 2
- **time** time vector of length M
- mcmopts dict of mcmc parameters

default mcmc options: mcmcopts = {"iter":1*(10**4), "nchains":4, "vpriorvar":1,

```
"burnin":np.minimum(5*(10**3),2*(10**4)//2), "alpha0":0.1, "beta0":0.1, "alpha":1, "beta":1, "h":0.01, "L":4, "f1propvar":0.0001, "f2propvar":0.0001, "L1propvar":0.3, "L2propvar":0.3, "npoints":200, "thin":1, "sampfreq":1, "initcoef":np.repeat(0,20), "nbasis":10, "basis":'fourier', "extrainfo":True}
```

Basis can be 'fourier' or 'legendre'

:rtype collection containing :return f2_warped: aligned f2 :return gamma: warping function :return v_coef: final v_coef :return psi: final psi :return sigma1: final sigma

if extrainfo :return theta_accept: accept of psi samples :return f2_accept: accept of f2 samples :return SSE: SSE :return gamma_mat: posterior gammas :return gamma_stats: posterior gamma stats :return xdist: phase distance posterior :return ydist: amplitude distance posterior)

J. D. Tucker, L. Shand, and K. Chowdhary. "Multimodal Bayesian Registration of Noisy Functions using Hamiltonian Monte Carlo", Computational Statistics and Data Analysis, accepted, 2021.

time_warping.pairwise_align_functions(f1, f2, time, omethod='DP2', lam=0, grid_dim=7)

This function aligns f2 to f1 using the elastic square-root slope (srsf) framework.

Usage: out = pairwise_align_functions(f1, f2, time) out = pairwise_align_functions(f1, f2, time, omethod, lam, grid_dim)

Parameters

- **f1** vector defining M samples of function 1
- **f2** vector defining M samples of function 2
- **time** time vector of length M
- **omethod** optimization method (DP, DP2, RBFGS) (default = DP)
- lam controls the elasticity (default = 0)
- grid_dim size of the grid, for the DP2 method only (default = 7)

:rtype list containing :return f2n: aligned f2 :return gam: warping function :return q2n: aligned q2 (srsf)

```
time_warping.rand(d0, d1, ..., dn)
```

Random values in a given shape.

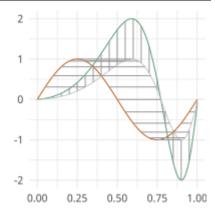
Note: This is a convenience function for users porting code from Matlab, and wraps *random_sample*. That function takes a tuple to specify the size of the output, which is consistent with other NumPy functions like *numpy.zeros* and *numpy.ones*.

Create an array of the given shape and populate it with random samples from a uniform distribution over [0, 1).

d0, d1, ..., dn [int, optional] The dimensions of the returned array, must be non-negative. If no argument is given a single Python float is returned.

out [ndarray, shape (d0, d1, ..., dn)] Random values.

random



FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS

Vertical and Horizontal Functional Principal Component Analysis using SRSF

moduleauthor:: J. 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, *stds*=*array*([-1, 0, 1]))

This function calculates horizontal functional principal component analysis on aligned data

Parameters

- **no** (*int*) number of components to extract (default = 3)
- stds number of standard deviations along gedoesic to compute (default = -1,0,1)

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 – principal 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, stds=array([-1., 0., 1.]), id=None, parallel=False, cores=-1)
           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)
                    • stds – number of standard deviations along gedoesic to compute (default = -1,0,1)
                    • parallel (bool) – run in parallel (default = F)
                    • cores (int) – number of cores for parallel (default = -1 (all))
               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, *stds*=array([-1, 0, 1]))

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)
- stds number of standard deviations along gedoesic to compute (default = -1,0,1)

Return type fdavpca object containing

Return q_pca srsf principal directions

Return f_pca functional principal directions

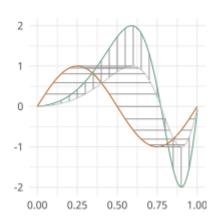
Return latent latent values

Return coef coefficients

Return U eigenvectors

plot()

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



ELASTIC FUNCTIONAL BOXPLOTS

```
Elastic Functional Boxplots
moduleauthor:: J. 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)
     plot()
           plot box plot and surface plot
           Usage: obj.plot()
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.

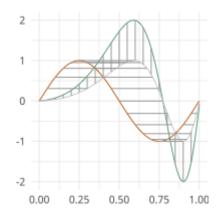
Parameters

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

plot()

plot box plot and surface plot

Usage: obj.plot()



FUNCTIONAL PRINCIPAL LEAST SQUARES

Partial Least Squares using SVD

moduleauthor:: J. 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
- \mathbf{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)

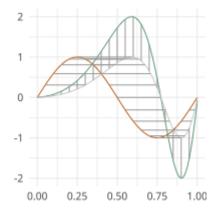
Return type numpy ndarray

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

class regression.elastic_logistic(f, y, time)

This class provides elastic logistic regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_logistic(f,y,time)

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
- alpha alpha parameter of model
- **beta** beta(t) of model
- fn aligned functions numpy ndarray of shape (M,N) of M functions with N samples
- qn aligned srvfs similar structure to fn
- gamma calculated warping functions
- **q** original training SRSFs
- **b** basis coefficients
- Loss logistic loss

Author: J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date: 29-Oct-2021

calc_model(B=None, lam=0, df=20, max_itr=20, cores=-1, smooth=False)

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

Parameters

- **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)

predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

Parameters

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed
- sparam number of times to run filter

class regression.elastic_mlogistic(f, y, time)

This class provides elastic multinomial logistic regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_mlogistic(f,y,time)

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
- alpha alpha parameter of model
- **beta** beta(t) of model
- fn aligned functions numpy ndarray of shape (M,N) of N functions with M samples
- qn aligned srvfs similar structure to fn
- gamma calculated warping functions
- **q** original training SRSFs
- **b** basis coefficients
- Loss logistic loss

Author: J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date: 29-Oct-2021

calc_model(*B=None*, *lam=0*, *df=20*, *max_itr=20*, *delta=0.01*, *cores=-1*, *smooth=False*)

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

Parameters

- **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)

predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

Parameters

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed
- **sparam** number of times to run filter

class regression.elastic_regression(f, y, time)

This class provides elastic regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_regression(f,y,time)

Parameters

- \mathbf{f} numpy ndarray of shape (M,N) of N functions with M samples
- y numpy array of N responses
- **time** vector of size M describing the sample points
- B optional matrix describing Basis elements
- alpha alpha parameter of model
- **beta** beta(t) of model
- fn aligned functions numpy ndarray of shape (M,N) of M functions with N samples
- qn aligned srvfs similar structure to fn
- gamma calculated warping functions
- **q** original training SRSFs
- **b** basis coefficients
- SSE sum of squared error

Author: J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date: 29-Oct-2021

calc_model(B=None, lam=0, df=20, max_itr=20, cores=-1, smooth=False)

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

- **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)

predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

Parameters

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed
- sparam number of times to run filter

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
- \boldsymbol{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 logistic loss

regression.logit_hessian(s, b, X, y)

calculates hessian of the logistic loss

- 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. $logit_loss(b, X, y)$

 $logistic loss function, returns Sum{-log(phi(t))}$

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

- alpha scalar
- beta numpy ndarray of shape (M,N) of N functions with M samples
- ullet time vector of size M describing the sample points
- \mathbf{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)

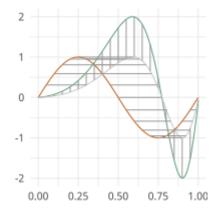
calculates optimal warping for function linear regression

Parameters

- beta numpy ndarray of shape (M,N) of M functions with N samples
- \bullet $\,$ 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
- alpha numpy scalar

Return type numpy array

Return gamma_new warping function



ELASTIC PRINCIPAL COMPONENT REGRESSION

Warping Invariant PCR Regression using SRSF

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

class pcr_regression.elastic_lpcr_regression(f, y, time)

This class provides elastic logistic pcr regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_lpcr_regression(f,y,time)

Parameters

- $\mathbf{f} (M,N)$ % matrix defining N functions of M samples
- y response vector of length N (-1/1)
- warp_data fdawarp object of alignment
- pca class dependent on fPCA method used object of fPCA

:param information :param alpha: intercept :param b: coefficient vector :param Loss: logistic loss :param PC: probability of classification :param ylabels: predicted labels

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

calc_model(*pca_method='combined'*, *no=5*, *smooth_data=False*, *sparam=25*, *parallel=False*)

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

Parameters

- pca_method string specifing 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 calculate in parallel (default = F)

predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

Parameters

• **newdata** (*dict*) – dict containing new data for prediction (needs the keys below, if None predicts on training data)

- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- y truth if available
- smooth smooth data if needed
- sparam number of times to run filter

class pcr_regression.elastic_mlpcr_regression(f, v, time)

This class provides elastic multinomial logistic per regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_mlpcr_regression(f,y,time)

Parameters

- $\mathbf{f} (M,N)$ % matrix defining N functions of M samples
- y response vector of length N
- Y coded label matrix
- warp_data fdawarp object of alignment
- pca class dependent on fPCA method used object of fPCA

:param information :param alpha: intercept :param b: coefficient vector :param Loss: logistic loss :param PC: probability of classification :param ylabels: predicted labels

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

calc_model(*pca_method='combined'*, *no=5*, *smooth_data=False*, *sparam=25*, *parallel=False*)

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 specifing 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 model in parallel (default = F)

predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions

- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed
- **sparam** number of times to run filter

class pcr_regression.elastic_pcr_regression(f, y, time)

This class provides elastic per regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_pcr_regression(f,y,time)

Parameters

- $\mathbf{f} (M,N)$ % matrix defining N functions of M samples
- y response vector of length N
- warp_data fdawarp object of alignment
- pca class dependent on fPCA method used object of fPCA
- alpha intercept
- **b** coefficient vector
- SSE sum of squared errors

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

calc_model(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

- **pca_method** string specifing 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)

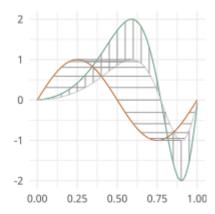
predict(newdata=None)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed

• **sparam** – number of times to run filter



ELASTIC GLM REGRESSION

Warping Invariant GML Regression using SRSF

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

class elastic_glm_regression.elastic_glm_regression(f, y, time)

This class provides elastic glm regression for functional data using the SRVF framework accounting for warping

Usage: obj = elastic_glm_regression(f,y,time)

Parameters

- $\mathbf{f} (M,N)$ % matrix defining N functions of M samples
- y response vector of length N
- time time vector of length M
- alpha intercept
- **b** coefficient vector
- **B** basis matrix
- lambda regularization parameter
- SSE sum of squared errors

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

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

- link string of link function ('linear', 'quadratic', 'cubic')
- **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)
- **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)

predict(newdata=None, parallel=True)

This function performs prediction on regression model on new data if available or current stored data in object Usage: obj.predict()

obj.predict(newdata)

Parameters

- **newdata** (*dict*) dict containing new data for prediction (needs the keys below, if None predicts on training data)
- $\mathbf{f} (M,N)$ matrix of functions
- **time** vector of time points
- **y** truth if available
- smooth smooth data if needed
- **sparam** number of times to run filter

```
elastic_glm_regression.rand(d0, d1, ..., dn)
```

Random values in a given shape.

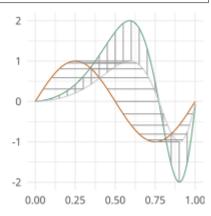
Note: This is a convenience function for users porting code from Matlab, and wraps *random_sample*. That function takes a tuple to specify the size of the output, which is consistent with other NumPy functions like *numpy.zeros* and *numpy.ones*.

Create an array of the given shape and populate it with random samples from a uniform distribution over [0, 1).

d0, **d1**, ..., **dn** [int, optional] The dimensions of the returned array, must be non-negative. If no argument is given a single Python float is returned.

```
out [ndarray, shape (d0, d1, ..., dn)] Random values.
```

random



ELASTIC FUNCTIONAL TOLERANCE BOUNDS

Functional Tolerance Bounds using SRSF

moduleauthor:: J. 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
- \mathbf{a} confidence level of tolerance bound (default = 0.05)
- \mathbf{p} coverage level of tolerance bound (default = 0.99)
- \mathbf{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.

- $\mathbf{x} (M,N)$ 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
- \mathbf{a} confidence level of tolerance bound (default = 0.05)
- \mathbf{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)

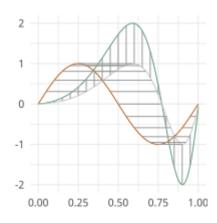
Computes a random wishart matrix

Parameters

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

Return type double

Return R matrix



CURVE REGISTRATION

statistic calculation for SRVF (curves) open and closed using Karcher Mean and Variance

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

class curve_stats.**fdacurve**(beta, mode='O', N=200, scale=False)

This class provides alignment methods for open and closed curves using the SRVF framework

Usage: obj = fdacurve(beta, mode, N, scale) :param beta: numpy ndarray of shape (n, M, N) describing N curves in R^M :param mode: Open ('O') or closed curve ('C') (default 'O') :param N: resample curve to N points :param scale: scale curve to length 1 (true/false) :param q: (n,T,K) matrix defining n dimensional srvf on T samples with K srvfs :param betan: aligned curves :param qn: aligned srvfs :param basis: calculated basis :param beta_mean: karcher mean curve :param q_mean: karcher mean srvf :param gams: warping functions :param v: shooting vectors :param C: karcher covariance :param s: pca singular values :param U: pca singular vectors :param coef: pca coefficients :param pca principal directions :param qun: cost function :param samples: random samples :param gamr: random warping functions :param cent: center :param scale: scale :param len: length of curve :param len_q: length of srvf :param mean_scale mean length :param mean_scale_q mean length srvf :param E: energy

Author: J. D. Tucker (JDT) < jdtuck AT sandia.gov > Date: 26-Aug-2020

karcher_cov()

This calculates the mean of a set of curves

karcher_mean(rotation=True, parallel=False, cores=-1, method='DP')

This calculates the mean of a set of curves :param rotation: compute optimal rotation (default = T) :param parallel: run in parallel (default = T) :param cores: number of cores for parallel (default = T) :param method: method to apply optimization (default="DP") options are "DP" or "RBFGS"

plot()

plot curve mean results

sample_shapes(no=3, numSamp=10)

Computes sample shapes from mean and covariance

Parameters

- **no** number of direction (default 3)
- **numSamp** number of samples (default 10)

$shape_pca(no=10)$

Computes principal direction of variation specified by no. N is Number of shapes away from mean. Creates 2*N+1 shape sequence

Parameters no – number of direction (default 3)

```
srvf_align(rotation=True, parallel=False, cores=-1, method='DP')
```

This aligns a set of curves to the mean and computes mean if not computed :param rotation: compute optimal rotation (default = T) :param parallel: run in parallel (default = T) :param cores: number of cores for parallel (default = T) :param method: method to apply optimization (default="DP") options are "DP" or "RBFGS"

```
curve_stats.randn(d0, d1, ..., dn)
```

Return a sample (or samples) from the "standard normal" distribution.

Note: This is a convenience function for users porting code from Matlab, and wraps *standard_normal*. That function takes a tuple to specify the size of the output, which is consistent with other NumPy functions like *numpy.zeros* and *numpy.ones*.

Note: New code should use the standard_normal method of a default_rng() instance instead; please see the random-quick-start.

If positive int_like arguments are provided, *randn* generates an array of shape (d0, d1, ..., dn), filled with random floats sampled from a univariate "normal" (Gaussian) distribution of mean 0 and variance 1. A single float randomly sampled from the distribution is returned if no argument is provided.

- **d0**, **d1**, ..., **dn** [int, optional] The dimensions of the returned array, must be non-negative. If no argument is given a single Python float is returned.
- **Z** [ndarray or float] A (d0, d1, ..., dn)-shaped array of floating-point samples from the standard normal distribution, or a single such float if no parameters were supplied.

standard_normal: Similar, but takes a tuple as its argument. normal: Also accepts mu and sigma arguments. Generator.standard_normal: which should be used for new code.

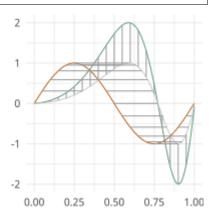
For random samples from $N(\mu, \sigma^2)$, use:

```
sigma * np.random.randn(...) + mu
```

```
>>> np.random.randn()
2.1923875335537315 # random
```

Two-by-four array of samples from N(3, 6.25):

```
>>> 3 + 2.5 * np.random.randn(2, 4)
array([[-4.49401501, 4.00950034, -1.81814867, 7.29718677], # random
[ 0.39924804, 4.68456316, 4.99394529, 4.84057254]]) # random
```



SRVF GEODESIC COMPUTATION

geodesic calculation for SRVF (curves) open and closed

moduleauthor:: J. 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)
- \mathbf{k} number of samples along path (Default = 5)

Return type numpy ndarray

Return utilde translated vector

 ${\tt geodesic.calc_alphadot}(\textit{alpha}, \textit{basis}, \textit{T=100}, \textit{k=5})$

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)
- \mathbf{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)
- \mathbf{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)
- \mathbf{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)
- \mathbf{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)
- \mathbf{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 geodisc distance for path straightening

Parameters

- beta numpy ndarray of shape (2,M) of M samples
- \mathbf{k} number of samples along path (Default = 5)

Return type numpy scalar

Return dist geodesic distance

geodesic.geod_sphere(beta1, beta2, k=5, scale=False, rotation=True, center=True)

This function calculates the geodesics 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
- \mathbf{k} number of samples along path (Default = 5)
- **scale** include length (Default = False)
- **rotation** include rotation (Default = True)
- **center** center curves at origin (Default = True)

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 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)
- \mathbf{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 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)
- \mathbf{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)
- \mathbf{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

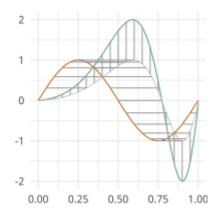
Parameters

- 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 paramenter
- **T** Number of samples of curve (Default = 100)
- \mathbf{k} number of samples along path (Default = 5)

Return type numpy scalar

Return alpha updated path of srvfs

Return beta updated path of curves



CHAPTER

TWELVE

UTILITY FUNCTIONS

Utility functions for SRSF Manipulations

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

utility_functions.SqrtMean(gam, parallel=False, cores=-1)

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
- **parallel** run in parallel (default = F)
- **cores** number of cores for parallel (default = -1 (all))

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

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

 $\verb|utility_functions.elastic_depth| (\textit{f}, \textit{time}, \textit{method} = \textit{'DP2'}, \textit{lam} = 0.0, \textit{parallel} = \textit{True})|$

calculates the elastic depth between functions in matrix f

Parameters

- **f** matrix of size MxN (M time points for N functions)
- **time** vector of size M describing the sample points
- method method to apply optimization (default="DP2") options are "DP", "DP2", "RBFGS"
- lam controls the elasticity (default = 0.0)

Return type scalar

Return amp amplitude depth

Return phase phase depth

utility_functions.elastic_distance(f1, f2, time, method='DP2', 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
- method method to apply optimization (default="DP2") options are "DP","DP2","RBFGS"
- 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)

 $\verb|utility_functions.f_to_srsf|(f, time, smooth = False)|$

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 tr L'AM / sqrt(tr L'BL 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
- \mathbf{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 descrbing 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='DP2', lam=0.0, grid_dim=7) 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 samples of second SRSF
- method method to apply optimization (default="DP2") options are "DP", "DP2", "RBFGS"
- lam controls the amount of elasticity (default = 0.0)
- grid_dim size of the grid, for the DP2 method only (default = 7)

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 samples of second SRSF
- q2 vector of size N or array of NxM samples 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()
- \mathbf{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=1)

This function smooths a collection of functions using a box filter

Parameters

- \mathbf{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 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

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

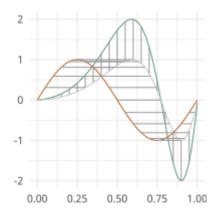
finds zero-crossing of optimal gamma, gam = s*gmax + (1-s)*gmin from elastic regression model

Parameters

- Y response
- **q** predicitve function
- bt basis function
- **time** time samples
- **y_max** maximum repsonse for warping function gmax
- **y_min** minimum response for warping function gmin
- gmax max warping function
- gmin min warping fucntion

Return type numpy array

Return gamma optimal warping function



CHAPTER

THIRTEEN

CURVE FUNCTIONS

functions for SRVF curve manipulations moduleauthor:: J. Derek Tucker <jdtuck@sandia.gov> curve_functions.Basis_Normal_A(q) Find Normal Basis **Parameters q** – numpy ndarray (n,T) defining T points on n dimensional SRVF :rtype list :return delg: basis 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, mode='O')

Parameters

- beta numpy ndarray of shape (2,M) of M samples
- mode Open ('O') or closed curve ('C') (default 'O')

Return type numpy ndarray

This function converts curve beta to srvf q

Return q srvf of curve

Return lenb length of curve

Return leng length of srvf

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

finds zero-crossing of optimal gamma, gam = s*gmax + (1-s)*gmin from elastic curve regression model

Parameters

- Y response
- beta predicitve function
- bt basis function
- y_max maximum repsonse for warping function gmax
- **y_min** minimum response for warping function gmin
- gmax max warping function
- gmin min warping fucntion

Return type numpy array

Return gamma optimal warping function

Return O hat rotation matrix

curve_functions.elastic_distance_curve(beta1, beta2, closed=0, rotation=True, scale=False, method='DP')

Calculates the two elastic distances between two curves :param beta1: numpy ndarray of shape (2,M) of M samples :param beta2: numpy ndarray of shape (2,M) of M samples :param closed: open (0) or closed (1) curve (default=0) :param rotation: compute optimal rotation (default=True) :param scale: include scale (default=False) :param method: method to apply optimization (default="DP") options are "DP" or "RBFGS"

Return type tuple

Return dist shape distance

Return dx phase distance

curve_functions.elastic_shooting(q1, v, mode=0)

Calculates shooting vector from v to q1

Parameters

- q1 vector of srvf
- **v** shooting vector
- mode closed or open (1/0)

:rtype numpy ndarray :return q2n: vector of srvf

curve_functions.elastic_shooting_vector(q1, q2, mode=0)

Calculates shooting between two srvfs

Parameters

- q1 vector of srvf
- q2 vector of srvf
- mode closed or open (1/0)

:rtype numpy ndarray :return v: shooting vector :return d: distance :return q2n: aligned srvf

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, allow_reflection=False, only_xy=False)

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
- **allow_reflection** bool indicating if reflection is allowed (i.e. if the determinant of the optimal rotation can be -1)
- only_xy bool indicating if rotation should only be allowed in the first two dimensions of the space

Return type numpy ndarray

Return q2new optimal rotated q2 to q1

Return R rotation matrix

curve_functions.find_rotation_and_seed_coord(beta1, beta2, closed=0, rotation=True, method='DP')
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
- **closed** Open (0) or Closed (1)
- **rotation** find rotation (default=True)
- method method to apply optimization (default="DP") options are "DP" or "RBFGS"

Return type numpy ndarray

Return beta2new optimal aligned beta2 to beta1

Return q2best optimal aligned q2 to q1

Return Rbest rotation matrix

Return gamIbest warping function

curve_functions.find_rotation_and_seed_q(q1, q2, closed=0, rotation=True, method='DP')

This function returns a candidate list of optimally oriented and registered (seed) srvs w.r.t. q1

Parameters

- q1 numpy ndarray of shape (2,M) of M samples
- **q2** numpy ndarray of shape (2,M) of M samples
- closed Open (0) or Closed (1)
- rotation find rotation (default=True)
- method method to apply optimization (default="DP") options are "DP" or "RBFGS"

Return type numpy ndarray

Return q2best optimal aligned q2 to q1

Return Rbest rotation matrix

Return gamIbest warping function

 $curve_functions.find_rotation_and_seed_unique(q1, q2, closed=0, rotation=True, method='DP')$

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
- closed Open (0) or Closed (1)
- **rotation** find rotation (default=True)
- method method to apply optimization (default="DP") options are "DP" or "RBFGS"

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 Orthogonlization 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 orthogonlized basis

curve_functions.group_action_by_gamma(q, gamma)

This function reparamerized 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 reparatermized srvf

$\verb|curve_functions.group_action_by_gamma_coord|(f, gamma)|$

This function reparamerized 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 reparatermized curve

curve_functions.innerprod_q2(q1, q2)

This function calculates the inner product in srvf space

- 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, closed=0, method='DP')

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
- closed open (0) or closed (1) curve
- method method to apply optimization (default="DP") options are "DP" or "RBFGS"

Return type numpy ndarray

Return v shooting vectors

Return dist distance

 $\verb|curve_functions.optimum_reparam_curve| (q1, q2, lam=0.0, method='DP')|$

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 samples of second SRVF
- lam controls the amount of elasticity (default = 0.0)
- method method to apply optimization (default="DP") options are "DP" or "RBFGS"

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

- 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 prepcoessed a curve beta to set of closed curves

Parameters

- beta numpy ndarray of shape (2,M) of M samples
- \mathbf{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, scale=1)

This function converts srvf to beta

Parameters

- **q** numpy ndarray of shape (n,M) of M samples
- scale scale of curve

Return type numpy ndarray

Return beta parameterized curve

curve_functions.resamplecurve(x, N=100, time=None, mode='O')

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)
- **time** timing vector (Default=None)
- mode Open ('O') or closed curve ('C') (default 'O')

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

 $\verb|curve_functions.shift_f(f, tau)|$

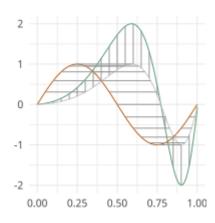
shifts a curve f by tau

Parameters

- \mathbf{f} numpy ndarray of shape (2,M) of M samples
- tau scalar

Return type numpy ndarray

Return fn shifted curve



CHAPTER

FOURTEEN

UMAP EFDA METRICS

Distance metrics for functions and curves in R^n for use with UMAP (https://github.com/lmcinnes/umap)

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

umap_metric.efda_distance(q1, q2)

"calculates the distances between two curves, where q2 is aligned to q1. In other words calculates the elastic distances/ This metric is set up for use with UMAP or t-sne from scikit-learn

Parameters

- q1 vector of size N
- q2 vector of size N

Return type scalar

Return dist amplitude distance

umap_metric.efda_distance_curve(beta1, beta2, closed)

"calculates the distances between two curves, where beta2 is aligned to beta1. In other words calculates the elastic distance. This metric is set up for use with UMAP or t-sne from scikit-learn

Parameters

- beta1 vector of size n*M
- beta2 vector of size n*M
- closed -
- (0) if open curves and (1) if closed curves

Return type scalar

Return dist shape distance

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