
fdasrsf Documentation

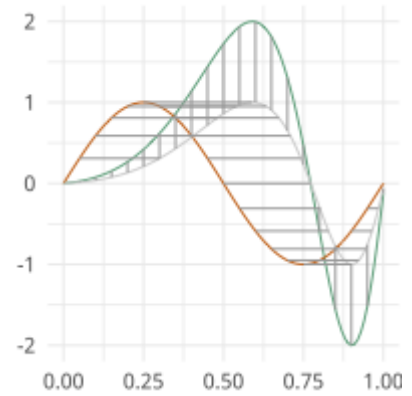
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J. Derek Tucker

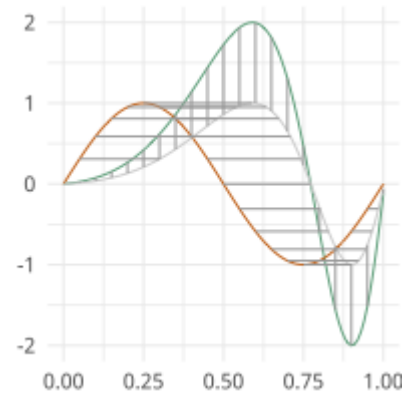
Jul 05, 2024

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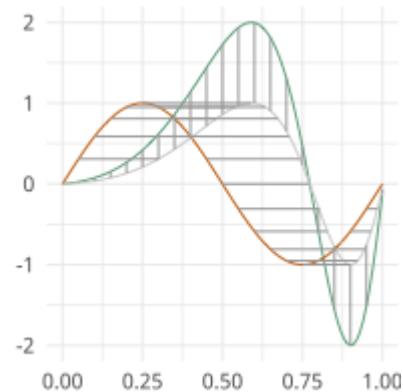


A python package for functional data analysis using the square root slope framework and curves using the square root velocity framework which performs pair-wise and group-wise alignment as well as modeling using functional component analysis and regression.



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)
```

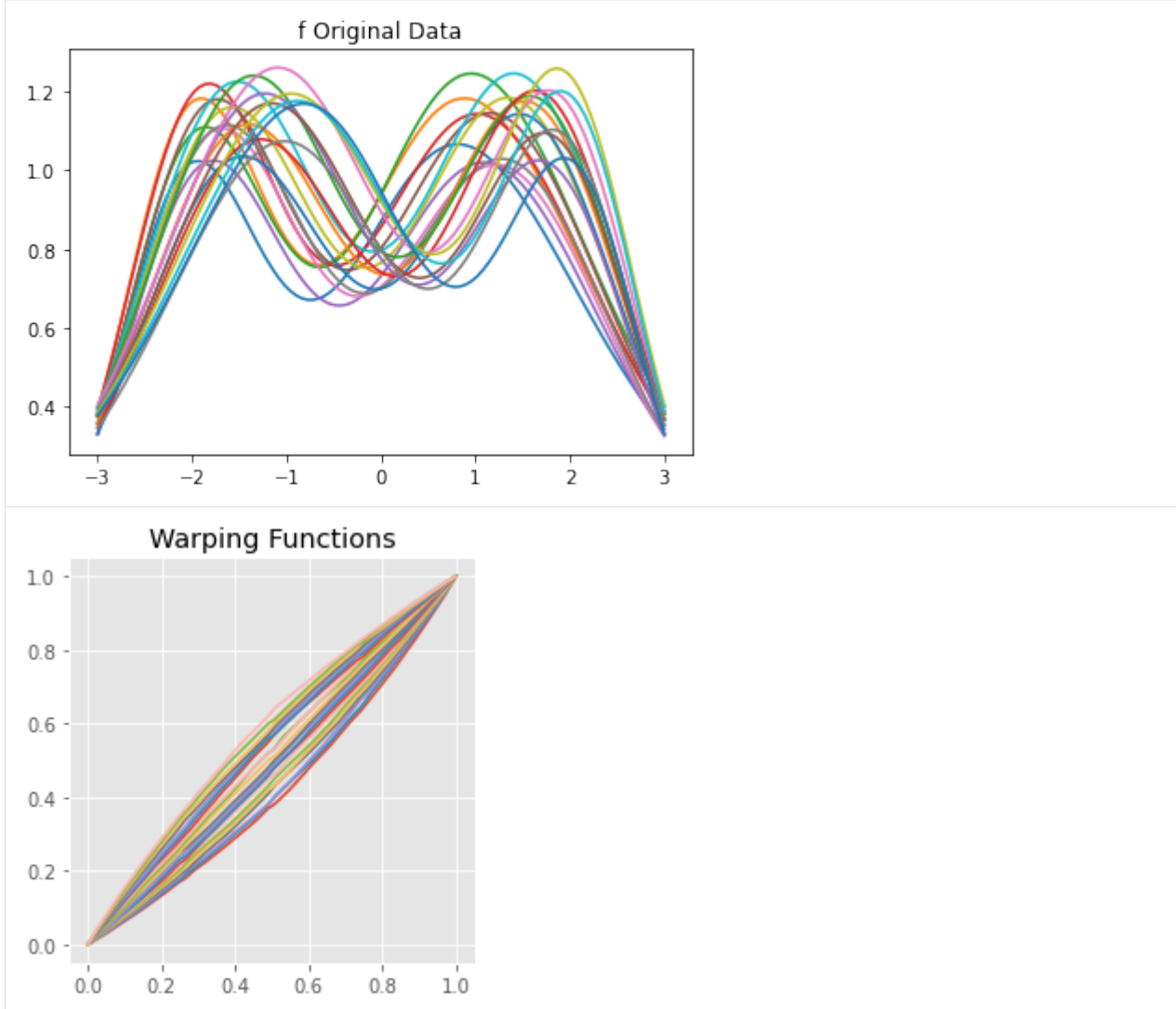
Next we will align the functions using the elastic framework

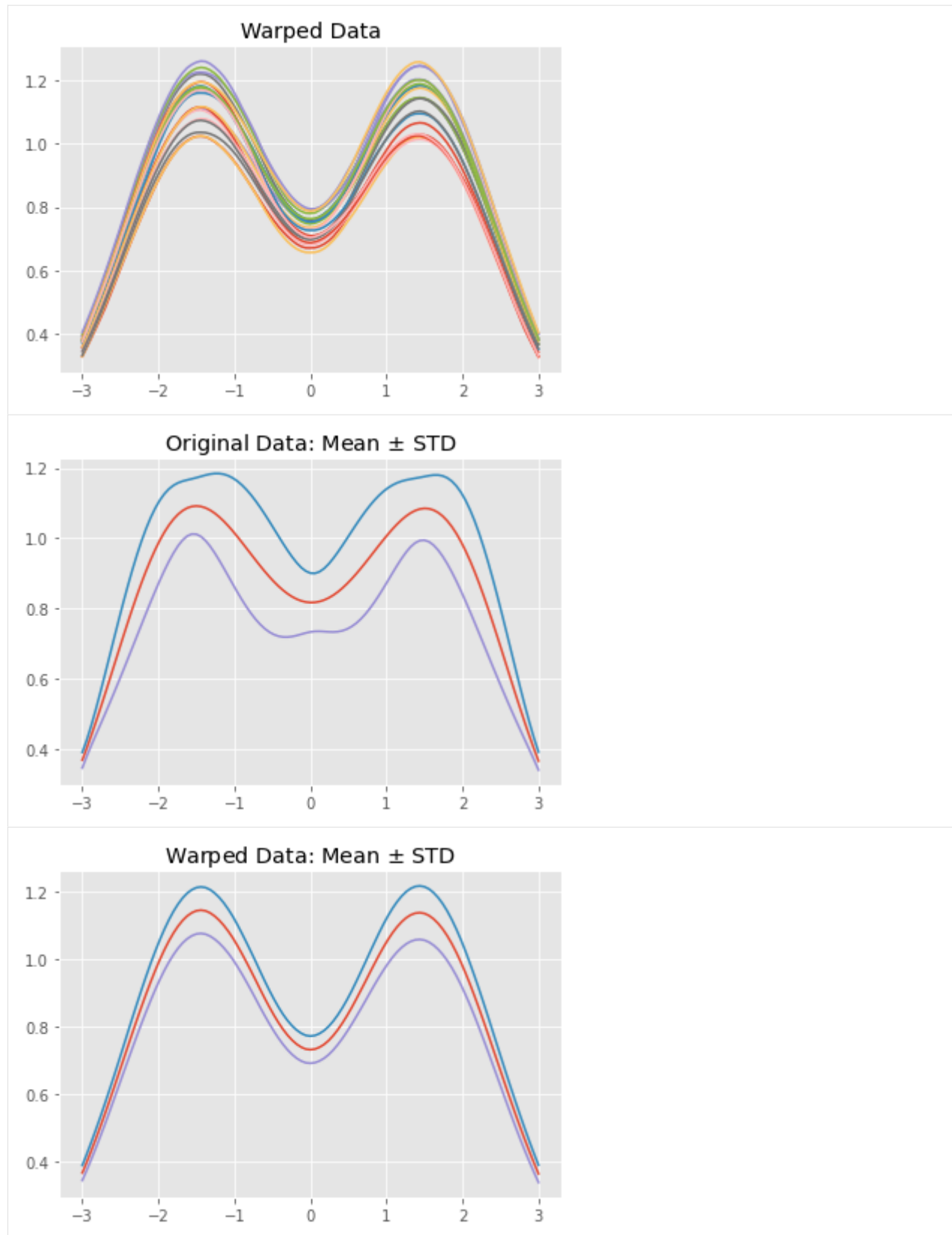
```
[4]: obj.srsf_align(parallel=True)

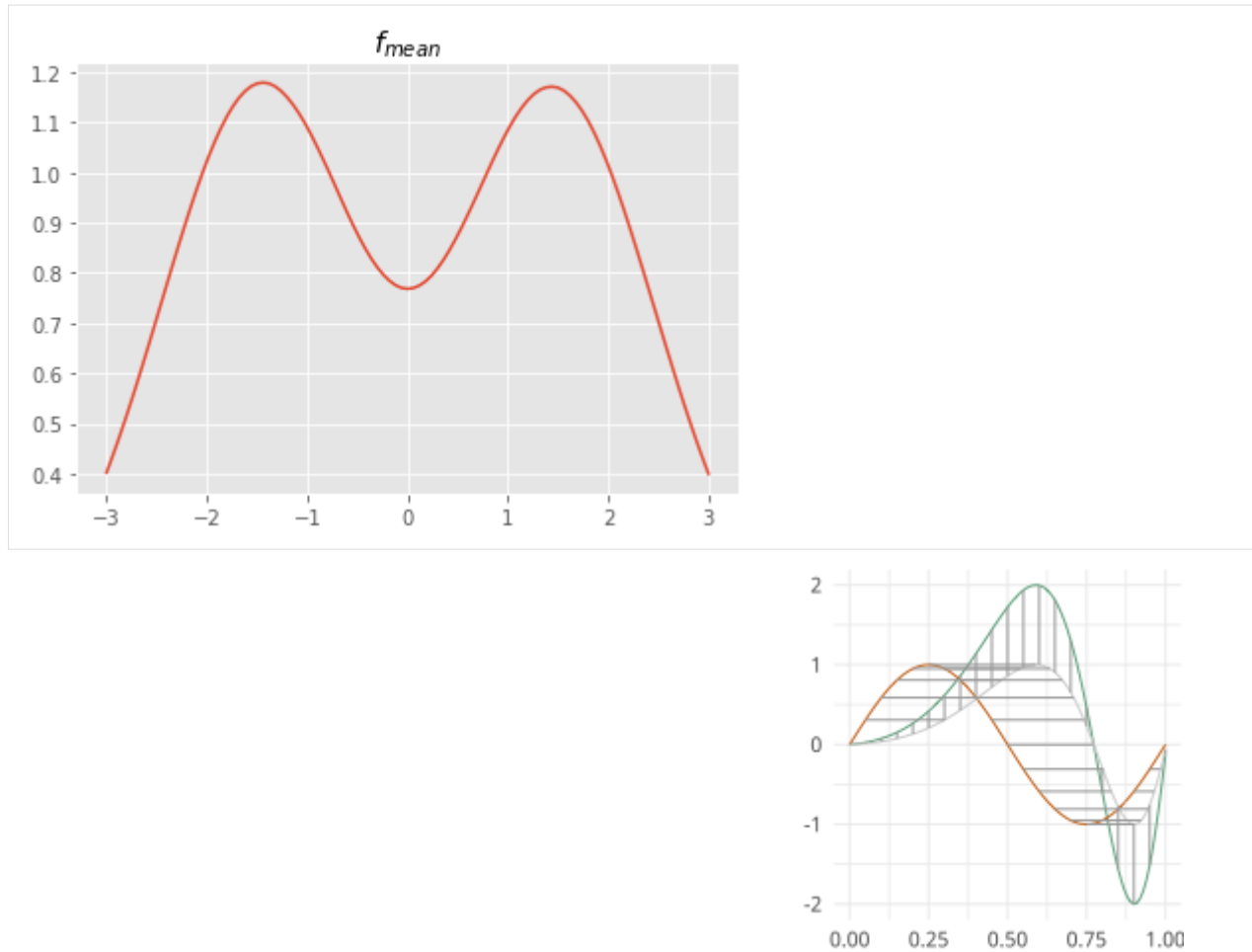
Initializing...
Compute Karcher Mean of 21 function in SRSF space...
updating step: r=1
updating step: r=2
```

Display plots demonstrating the alignment

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







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
```

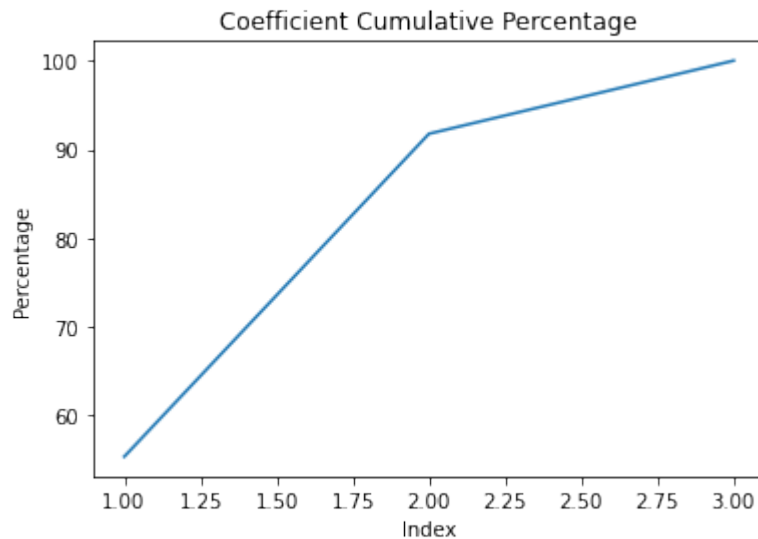
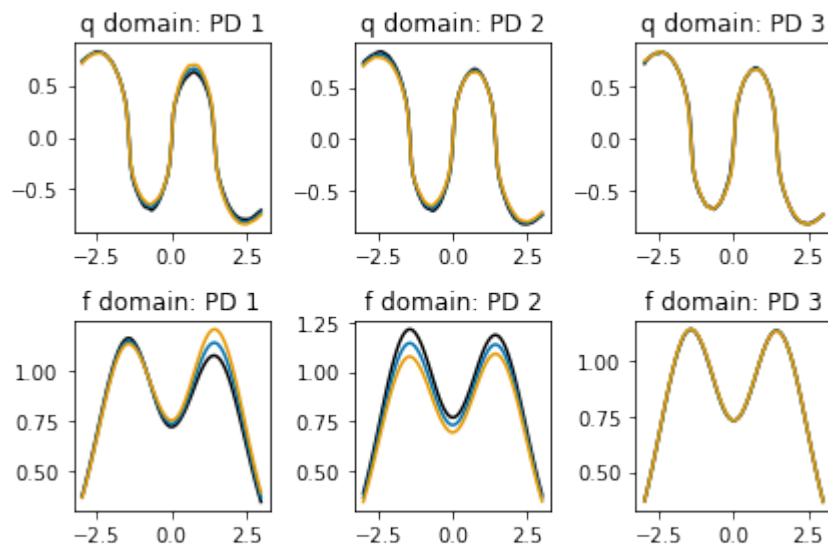
1.2.1 Vertical fPCA

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.fdapca(obj)
     vpca.calc_fpca(no=3)
```

We then can plot the principal directions

```
[4]: vpca.plot()
```



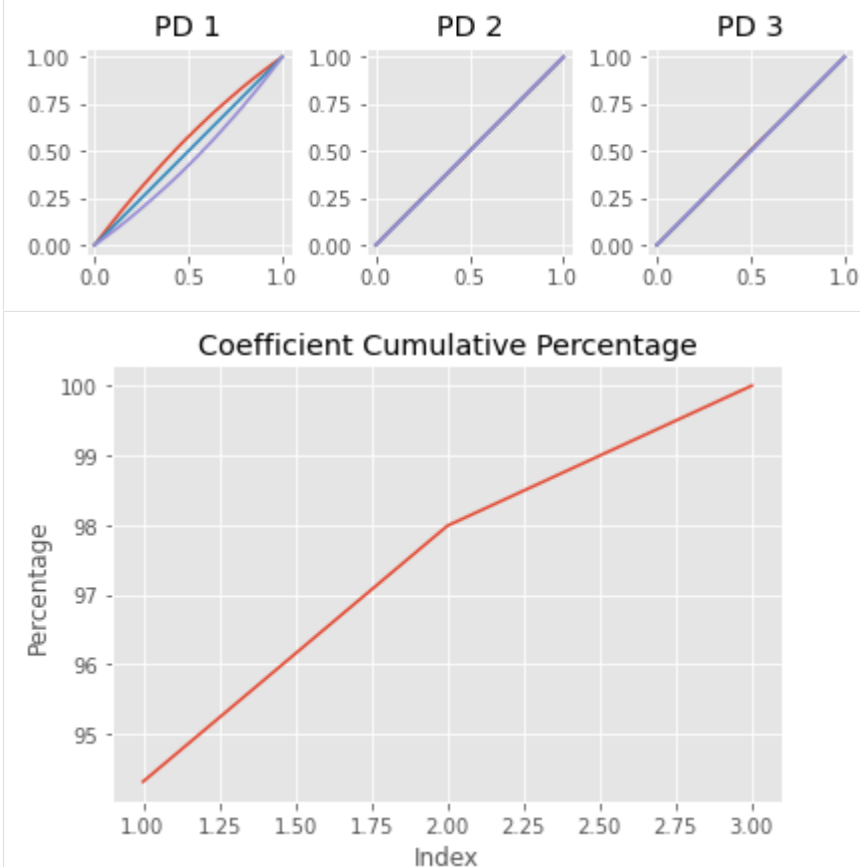
1.2.2 Horizontal fPCA

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

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



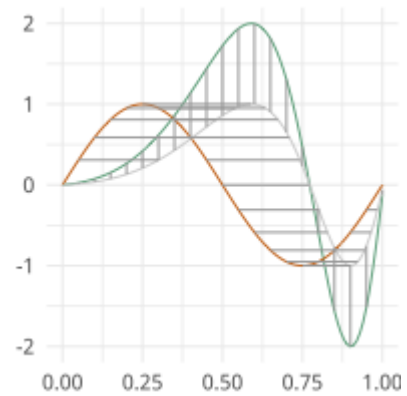
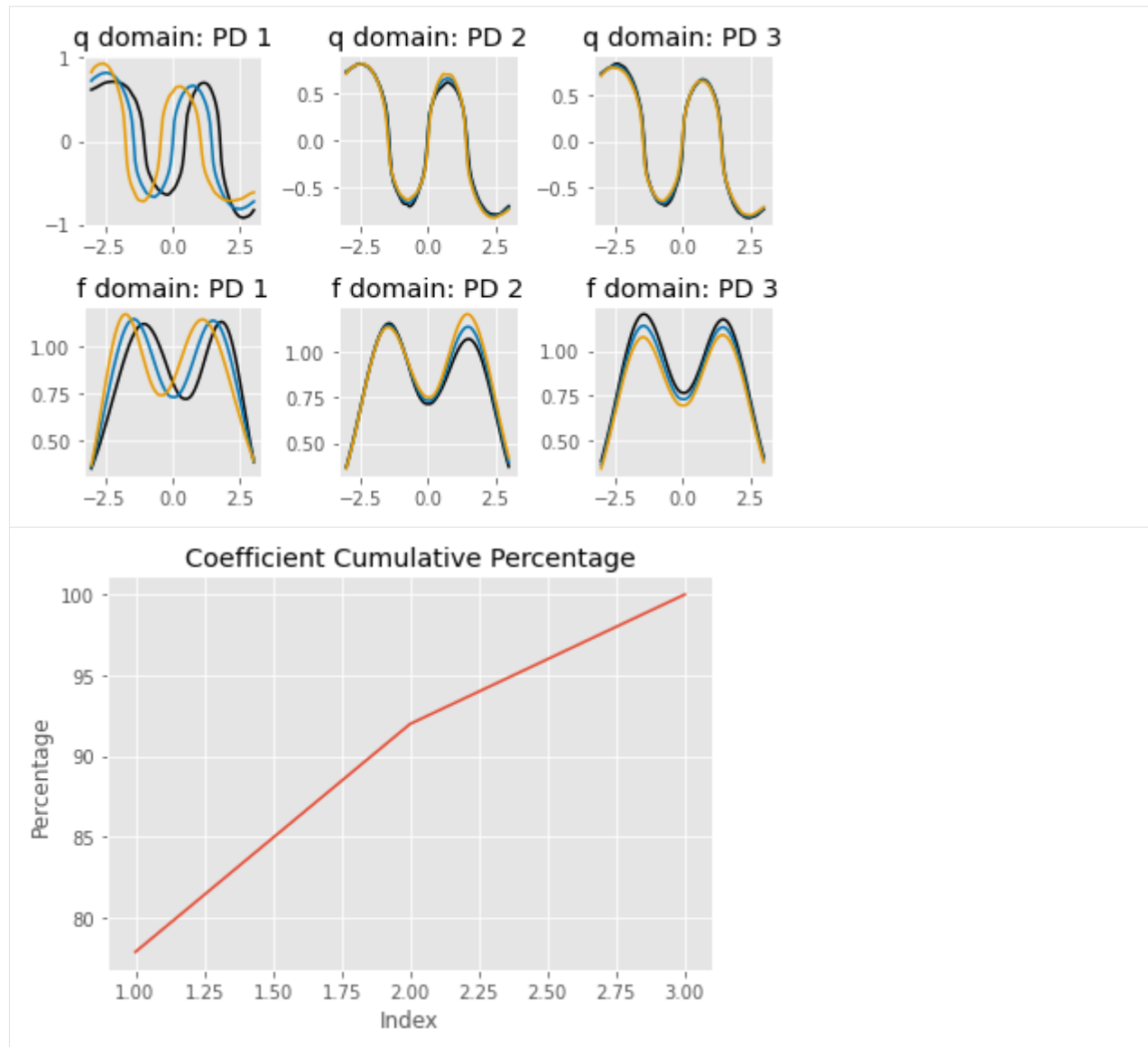
1.2.3 Joint fPCA

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 Multivariate Functional Example

This notebook will show how to use the `fdasrsf` package to align and statistically analyze a set of multivariate functions using the SRVF framework

1.3.1 Load Packages

We will load the required packages and the example data set (MPEG7)

```
[1]: import fdasrsf as fs
import matplotlib.pyplot as plt
import numpy as np
data = np.load('../bin/gait_data.npz', allow_pickle=True)
f = data['f']
g = data['g']
time = data['time']
```

Now we will construct a 2-D array of a set of 1-D functions from the gait data

```
[2]: M,K = f.shape

beta = np.zeros((2,M,K))
beta[0,:,:] = f
beta[1,:,:] = g
```

1.3.2 Analyze

We now will construct a `fdacurve` object

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

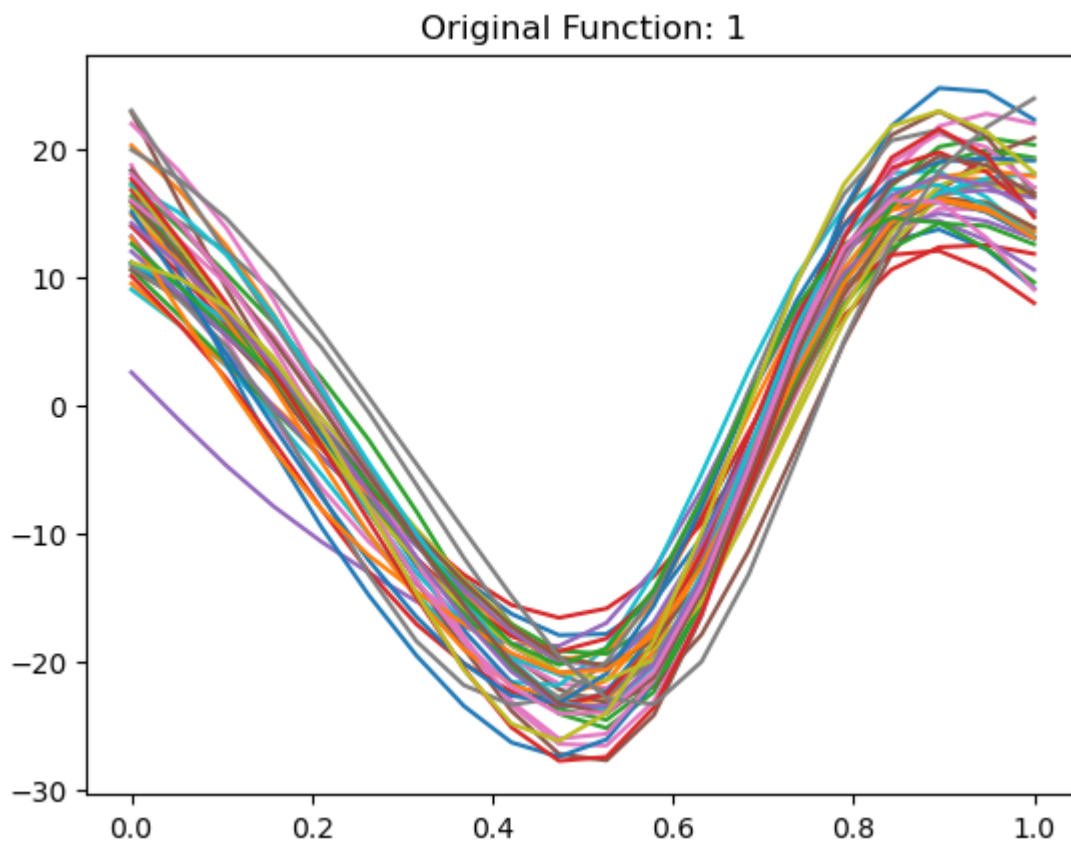
Next, find the Karcher mean and align the curves to the mean

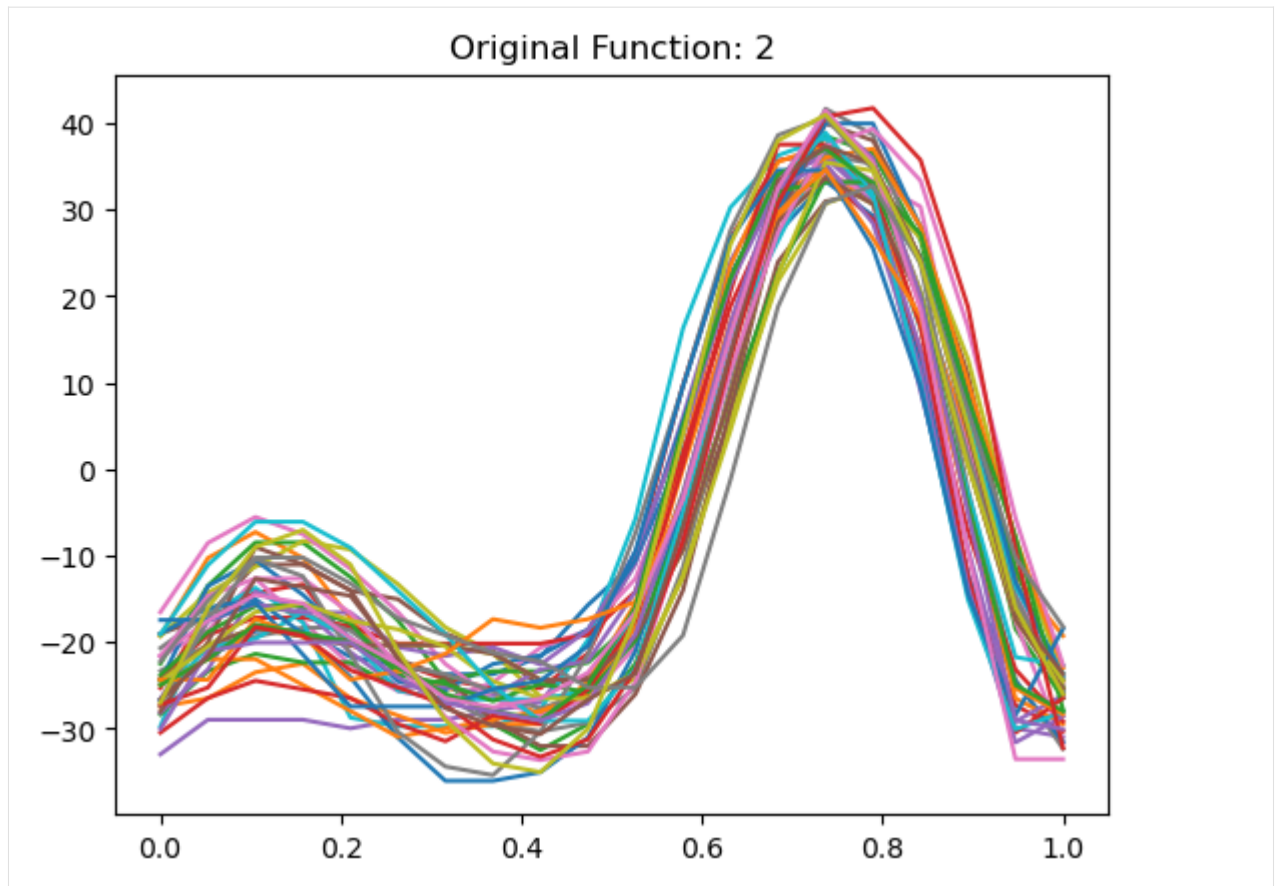
```
[ ]: obj.karcher_mean(rotation=False)
obj.srvf_align(rotation=False)

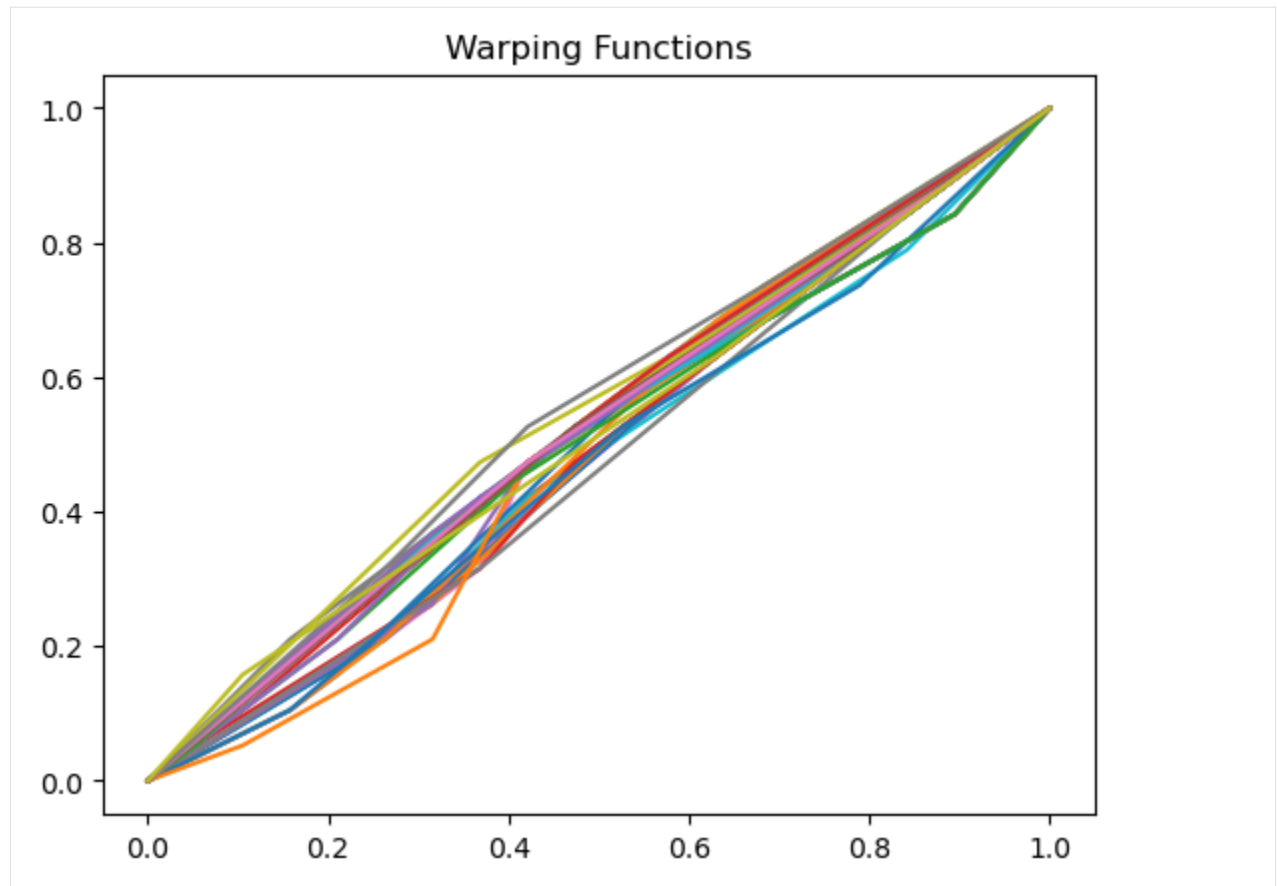
Computing Karcher Mean of 39 curves in SRVF space with lam=0
updating step: 1
updating step: 2
updating step: 3
updating step: 4
updating step: 5
updating step: 6
updating step: 7
updating step: 8
updating step: 9
updating step: 10
updating step: 11
```

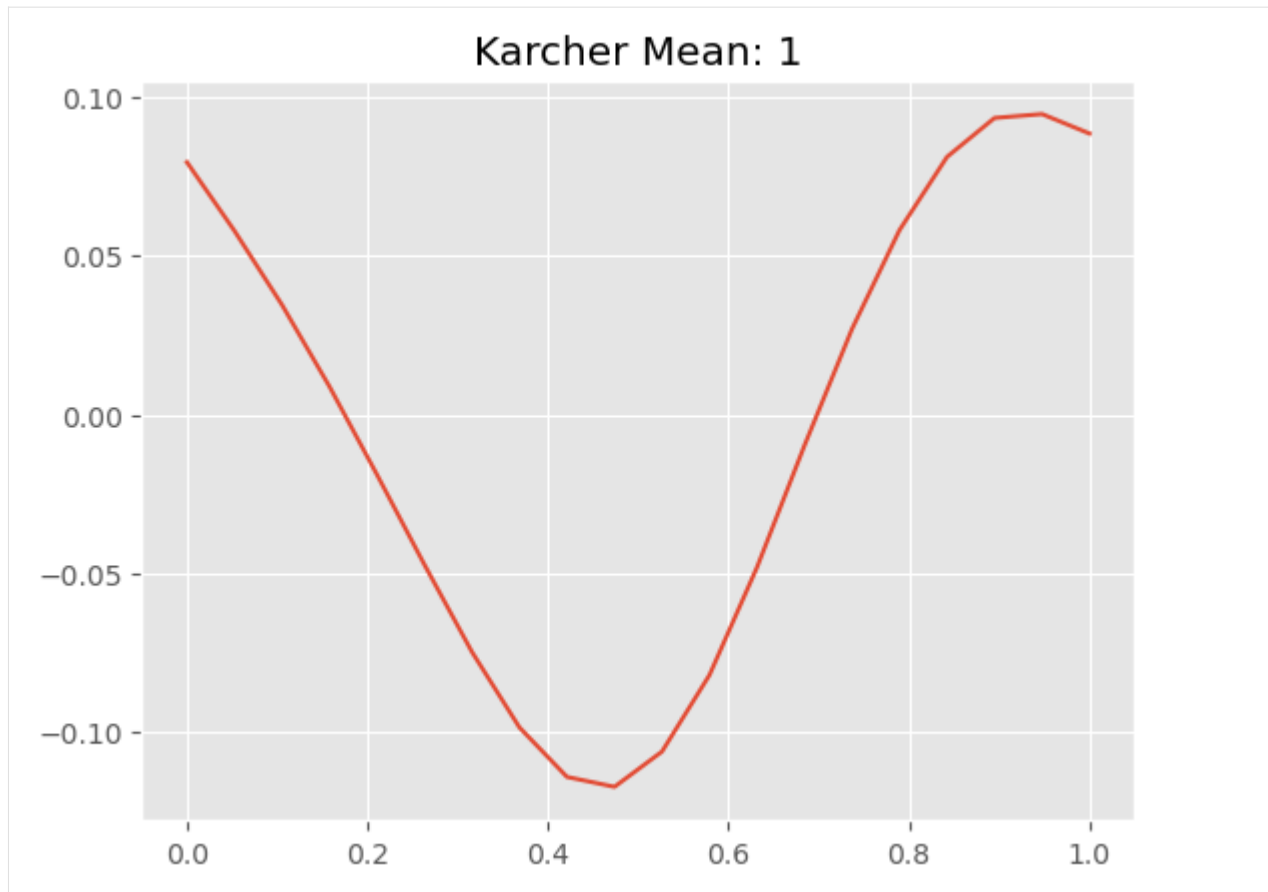
We will now plot the results

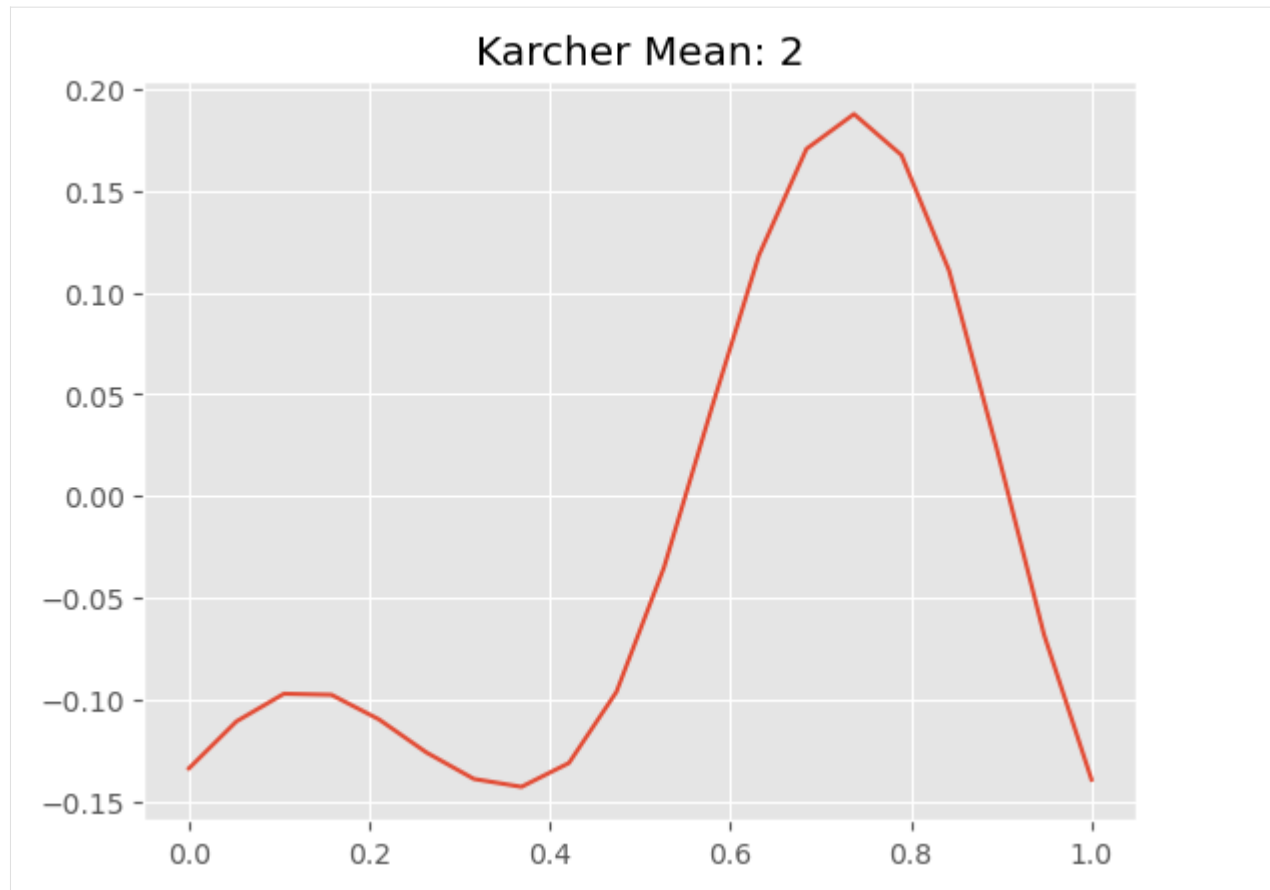
```
[ ]: obj.plot(multivariate=True)
```

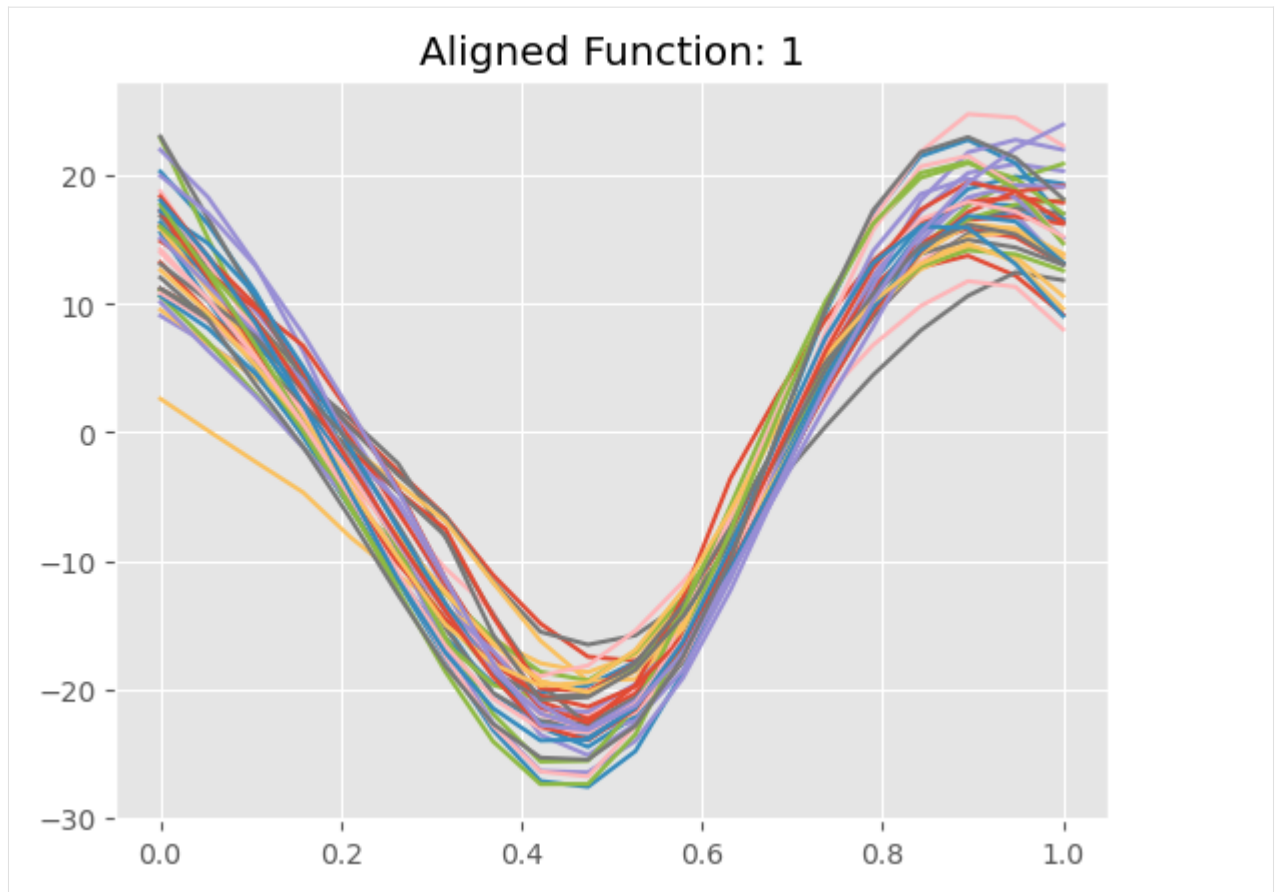


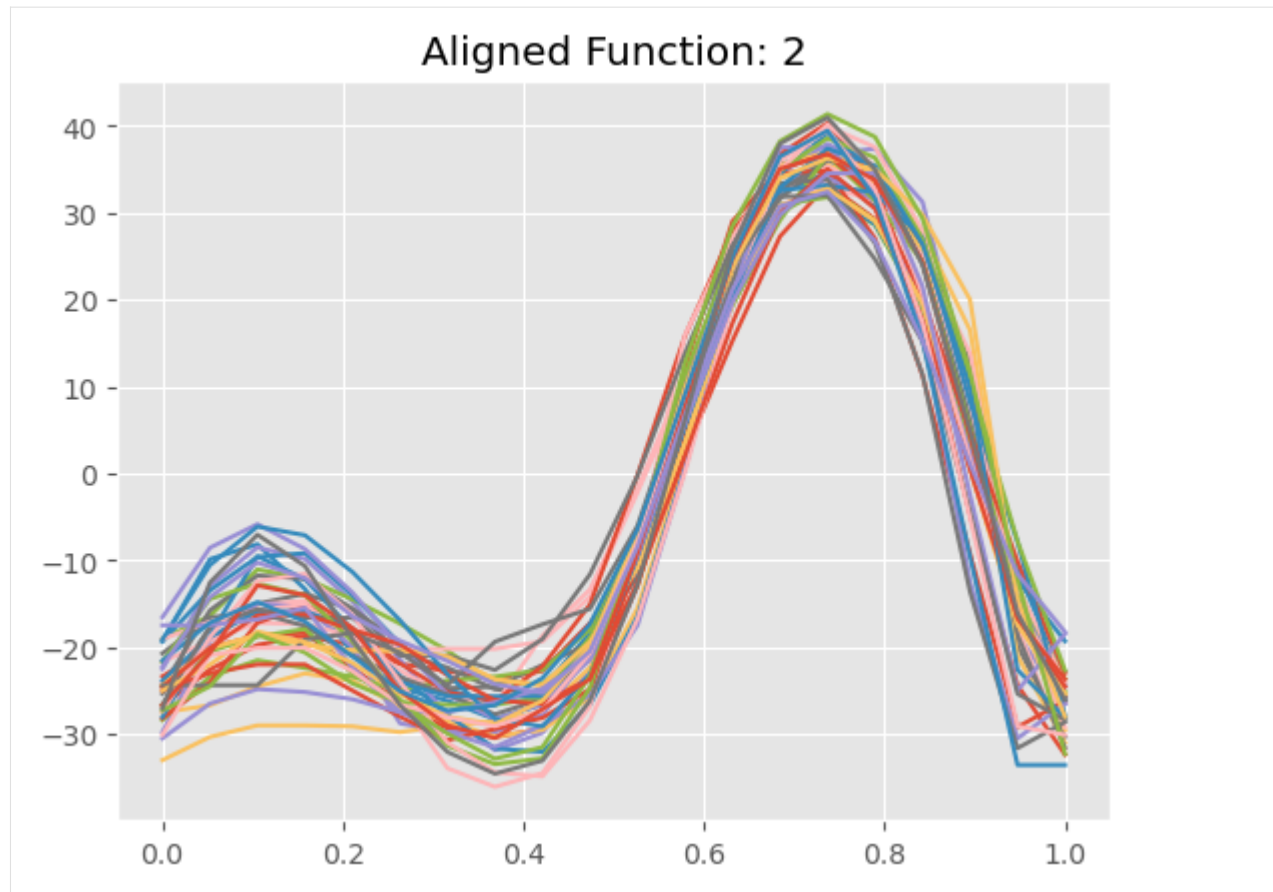




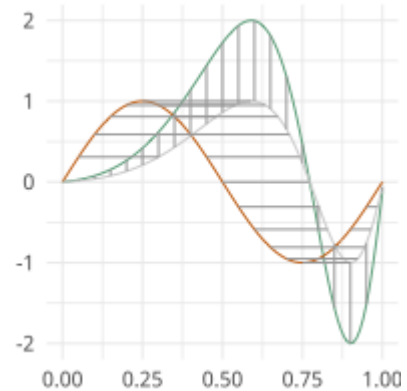








```
[ ]:
```



1.4 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()

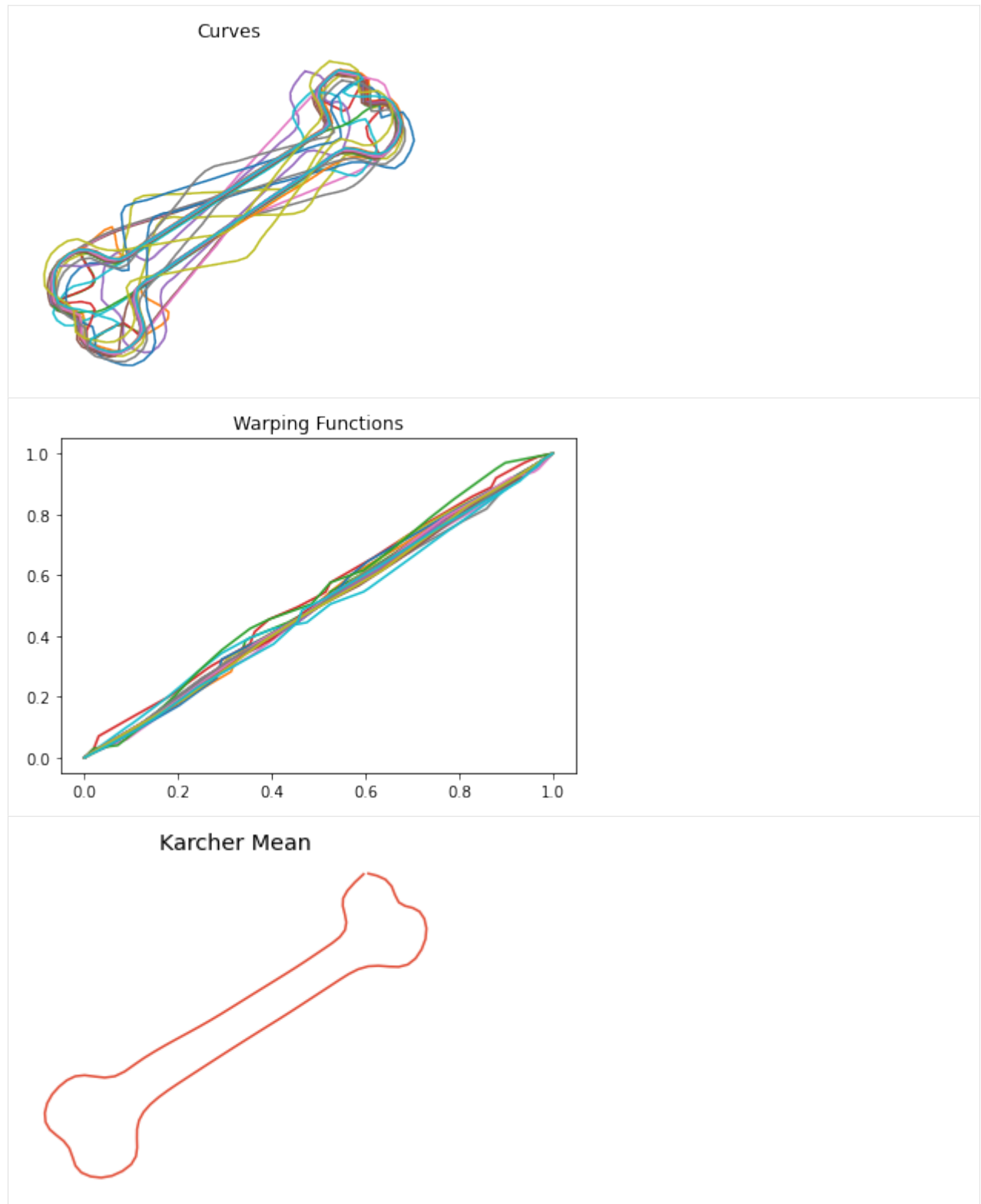
Computing Karcher Mean of 20 curves in SRVF space..
updating step: 1
updating step: 2
updating step: 3
updating step: 4
updating step: 5
updating step: 6
updating step: 7
```

We then can align the curves to the karcher mean

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

Plot the results

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



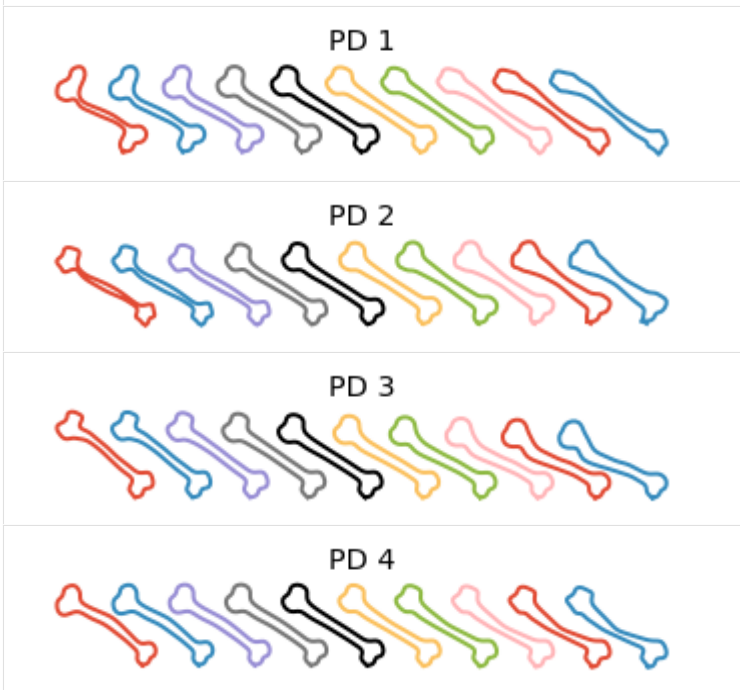
1.4.1 Shape PCA

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

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

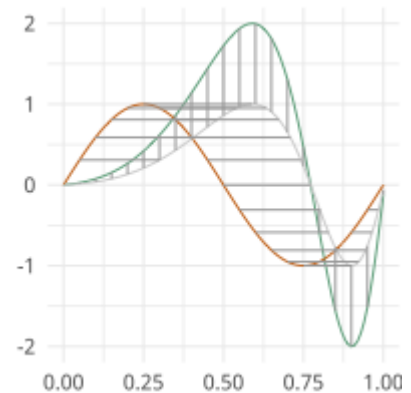
Plot the principal directions

```
[8]: obj.plot_pca()
```





API REFERENCE



2.1 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 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** – Karcher 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, pen='roughness', 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)

Parameters

- **mu** – vector of function to align to
- **omethod** – optimization method (DP, DP2, RBFGS, cRBFGS) (default = DP2)
- **smoothdata** (*bool*) – Smooth the data using a box filter (default = F)
- **parallel** – run in parallel (default = F)
- **lam** (*double*) – controls the elasticity (default = 0)
- **penalty** – penalty type (default="roughness") options are "roughness", "l2gam", "l2psi", "geodesic". Only roughness implemented in all methods. To use others method needs to be "RBFGS" or "cRBFGS"
- **cores** – number of cores for parallel (default = -1 (all))
- **grid_dim** – size of the grid, for the DP2 method only (default = 7)

plot()

plot functional alignment results

Usage: obj.plot()

srsf_align(*method='mean', omethod='DP2', center=True, smoothdata=False, MaxIter=20, parallel=False, lam=0.0, pen='roughness', cores=-1, grid_dim=7, verbose=True*)

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, RBFSG, cRBFSG) (default = DP2)
- **center** – center warping functions (default = T)
- **smoothdata** (*bool*) – Smooth the data using a box filter (default = F)
- **MaxIter** – Maximum number of iterations (default = 20)
- **parallel** – run in parallel (default = F)
- **lam** (*double*) – controls the elasticity (default = 0)
- **penalty** – penalty type (default=“roughness”) options are “roughness”, “l2gam”, “l2psi”, “geodesic”. Only roughness implemented in all methods. To use others method needs to be “RBFSG” or “cRBFSG”
- **cores** – number of cores for parallel (default = -1 (all))
- **grid_dim** – size of the grid, for the DP2 method only (default = 7)
- **verbose** – print status output (default = T)

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.pairwise_align_bayes(f1i, 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)

Parameters

- **f1i** – vector defining M samples of function 1
- **f2i** – vector defining M samples of function 2
- **time** – time vector of length M
- **mcmcopts** – 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 measurement 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 infity-HMC algorithm is used to explore both local and global structure in the posterior distribution.

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

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: mcmopts = {"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,pen='roughness',
grid_dim=7)
```

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

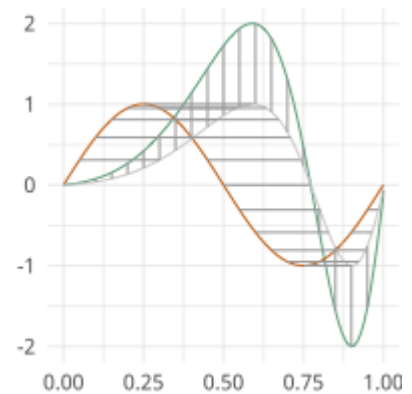
Usage: `out = pairwise_align_functions(f1, f2, time)`

```
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, cRBFGS) (default = DP)
- **lam** – controls the elasticity (default = 0)
- **penalty** – penalty type (default="roughness") options are "roughness", "l2gam", "l2psi", "geodesic". Only roughness implemented in all methods. To use others method needs to be "RBFGS" or "cRBFGS"
- **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)



2.2 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, var_exp=None, 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)
- **var_exp** – compute no based on value percent variance explained (example: 0.95)
- **stds** – number of standard deviations along geodesic 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()

project(f)
project new data onto fPCA basis
Usage: obj.project(f)

Parameters
f – numpy array (MxN) of N functions on M time

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, var_exp=None, 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)

- **var_exp** – compute no based on value percent variance explained (example: 0.95)
- **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 joint fPCA result

Usage: obj.plot()

project(f)

project new data onto fPCA basis

Usage: obj.project(f)

Parameters

f – numpy array (MxN) of N functions on M time

class fPCA.fdajpcah(fdawarp)

This class provides joint fPCA using the SRVF framework using MFPCA

Usage: obj = fdajpcah(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_q** – eigenvectors for q
- **U_h** – eigenvectors for gam
- **C** – scaling value

- **stds** – geodesic directions

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 06-April-2024

calc_fpca(*var_exp=0.99, stds=array([-1., 0., 1.]), id=None, parallel=False, cores=-1, srsf=True*)

This function calculates joint functional principal component analysis on aligned data

Parameters

- **var_exp** – compute no based on value percent variance explained (default: None)
- **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))
- **U_q** – eigenvectors for q
- **U_h** – eigenvectors for gam

Return type

fdajpcah object of numpy ndarray

Return q_pca

srsf principal directions

Return f_pca

functional principal directions

Return latent

latent values

Return coef

coefficients

plot()

plot plot elastic joint fPCA result

Usage: obj.plot()

project(f)

project new data onto fPCA basis

Usage: obj.project(f)

Parameters

f – numpy array (MxN) of N functions on M time

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
- **new_coef** – principal coefficients of new data

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

calc_fpca(*no=3, var_exp=None, 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)
- **var_exp** – compute no based on value percent variance explained (example: 0.95)
- **id** (*int*) – point to use for $f(0)$ (default = midpoint)
- **stds** – number of standard deviations along geodesic 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()

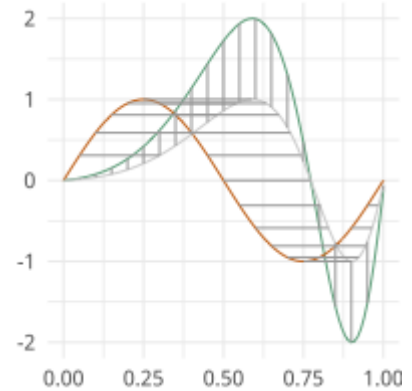
project(f)

project new data onto fPCA basis

Usage: obj.project(f)

Parameters

f – numpy array (MxN) of N functions on M time



2.3 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.

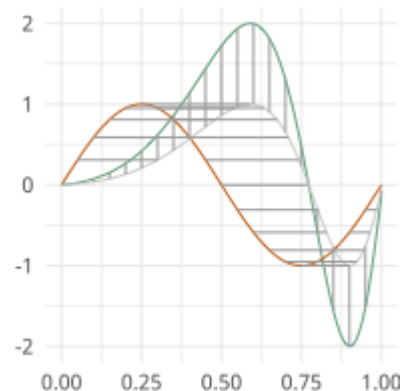
Parameters

- **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()`



2.4 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
- **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

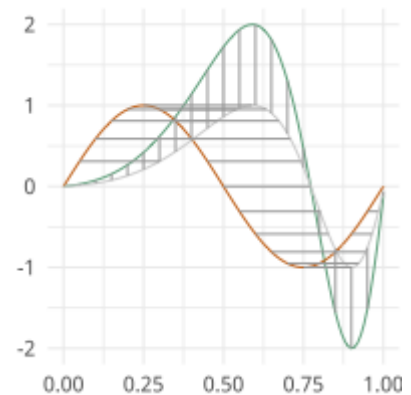
g weight function

Return alpha

smoothing value

Return values

singular values



2.5 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(newdata)`

Parameters

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

Parameters

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

- **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

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(newdata)

Parameters

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

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

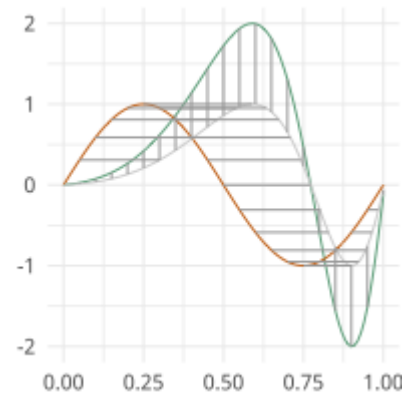
- **beta** – numpy ndarray of shape (M,N) of M functions with N samples
- **time** – vector of size N describing the sample points
- **q** – numpy ndarray of shape (M,N) of M functions with N samples
- **y** – numpy ndarray of shape (1,N) of M functions with N samples responses
- **alpha** – numpy scalar

Return type

numpy array

Return gamma_new

warping function



2.6 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

- **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
- **information**
- **alpha** – intercept
- **b** – coefficient vector
- **Loss** – logistic loss
- **PC** – probability of classification
- **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 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** – 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(newdata)

Parameters

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

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

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

Parameters

- **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
- **information**
- **alpha** – intercept
- **b** – coefficient vector
- **Loss** – logistic loss
- **PC** – probability of classification
- **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 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 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(newdata)

Parameters

- **newdata** (*dict*) – dict containing new data for prediction (needs the keys below, if None predicts on training data)
- **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 pcr regression for functional data using the SRVF framework accounting for warping

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

Parameters

- **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, var_exp=None, smooth_data=False, sparam=25, parallel=False, C=None*)

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

Parameters

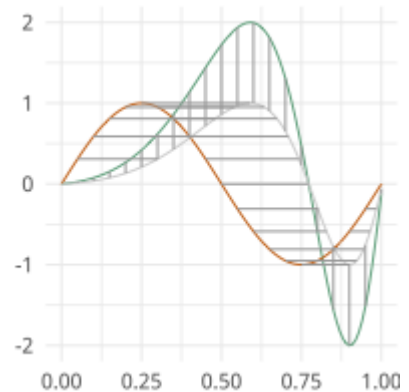
- **pca_method** – string specifying pca method (options = “combined”, “vert”, or “horiz”, default = “combined”)
- **no** – scalar specify number of principal components (default=5)
- **var_exp** – compute no based on value percent variance explained (example: 0.95)
- **smooth_data** – smooth data using 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, alpha=0.05*)

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

Parameters

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



2.7 Elastic Functional Changepoint

Elastic functional change point detection

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

```
class elastic_changepoint.elastic_amp_change_ff(f, time, smooth_data=False, sparam=25,
                                                use_warp_data=False, warp_data=None,
                                                parallel=False)
```

” This class provides elastic changepoint using elastic FDA. It is fully-functional and an extension of the methodology of Aue et al.

Usage: obj = elastic_amp_change_ff(f,time)

Parameters

- **f** – (M,N) % matrix defining N functions of M samples
- **time** – time vector of length M
- **warp_data** – aligned data (default: None)
- **Sn** – test statistic values
- **Tn** – max of test statistic
- **p** – p-value
- **k_star** – change point
- **values** – values of computed Brownian Bridges
- **dat_a** – data before changepoint
- **dat_b** – data after changepoint
- **warp_a** – warping functions before changepoint
- **warp_b** – warping functions after changepoint
- **mean_a** – mean function before changepoint
- **mean_b** – mean function after changepoint
- **warp_mean_a** – mean warping function before changepoint
- **warp_mean_b** – mean warping function after changepoint

Author : J. Derek Tucker <jdtuck AT sandia.gov> and Drew Yarger <anyarge AT sandia.gov> Date : 24-Aug-2022

```
compute(d=1000, h=0, M_approx=365, compute_epidemic=False)
```

Compute elastic change detection :param d: number of monte carlo iterations to compute p-value :param h: index of window type to compute long run covariance :param M_approx: number of time points to compute p-value :param compute_epidemic: compute epidemic changepoint model (default: False)

```
plot()
```

plot elastic changepoint results

Usage: obj.plot()

```
class elastic_changepoint.elastic_change(f, time, BBridges=None, use_BBridges=False,
                                          smooth_data=False, warp_data=None, use_warp_data=False,
                                          parallel=False, sparam=25)
```

” This class provides elastic changepoint using elastic fpca

Usage: `obj = elastic_change(f,time)`

Parameters

- **f** – (M,N) % matrix defining N functions of M samples
- **time** – time vector of length M
- **BBridges** – precomputed Brownian Bridges (default: None)
- **use_BBridges** – use precomputed Brownian Bridges (default: False)
- **warp_data** – aligned data (default: None)
- **Sn** – test statistic values
- **Tn** – max of test statistic
- **p** – p-value
- **k_star** – change point
- **values** – values of computed Brownian Bridges
- **dat_a** – data before changepoint
- **dat_b** – data after changepoint
- **warp_a** – warping functions before changepoint
- **warp_b** – warping functions after changepoint
- **mean_a** – mean function before changepoint
- **mean_b** – mean function after changepoint
- **warp_mean_a** – mean warping function before changepoint
- **warp_mean_b** – mean warping function after changepoin

Author : J. D. Tucker (JDT) <jdtuck AT sandia.gov> Date : 27-Apr-2022

compute(*pca_method='vert', pc=0.95, d=1000, compute_epidemic=False, n_pcs=5, preset_pcs=False*)

Compute elastic change detection

Parameters

- **pca_method** – string specifying pca method (options = “combined”, “vert”, or “horiz”, default = “combined”)
- **pc** – percentage of cumulative variance to use (default: 0.95)
- **compute_epidemic** – compute epidemic changepoint model (default: False)
- **n_pcs** – scalar specify number of principal components (default: 5)
- **preset_pcs** – use all PCs (default: False)

plot()

plot elastic changepoint results

Usage: `obj.plot()`

```
class elastic_changepoint.elastic_ph_change_ff(f, time, smooth_data=False, sparam=25,  
                                              use_warp_data=False, warp_data=None,  
                                              parallel=False)
```

” This class provides elastic changepoint using elastic FDA on warping functions. It is fully-functional and an extension of the methodology of Aue et al.

Usage: `obj = elastic_ph_change_ff(f,time)`

Parameters

- **f** – (M,N) % matrix defining N functions of M samples
- **time** – time vector of length M
- **warp_data** – aligned data (default: None)
- **Sn** – test statistic values
- **Tn** – max of test statistic
- **p** – p-value
- **k_star** – change point
- **values** – values of computed Brownian Bridges
- **dat_a** – data before changepoint
- **dat_b** – data after changepoint
- **warp_a** – warping functions before changepoint
- **warp_b** – warping functions after changepoint
- **mean_a** – mean function before changepoint
- **mean_b** – mean function after changepoint
- **warp_mean_a** – mean warping function before changepoint
- **warp_mean_b** – mean warping function after changepoint

Author : J. Derek Tucker <jdtuck AT sandia.gov> Date : 17-Nov-2022

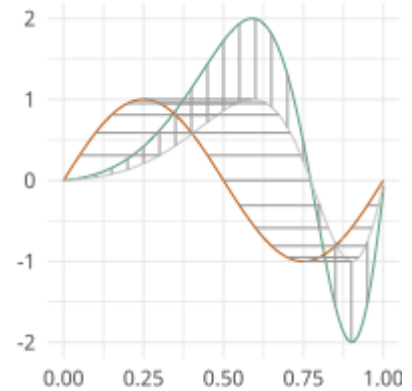
```
compute(d=1000, h=0, M_approx=365)
```

Compute elastic change detection :param d: number of monte carlo iterations to compute p-value :param h: index of window type to compute long run covariance :param M_approx: number of time points to compute p-value

```
plot()
```

plot elastic changepoint results

Usage: `obj.plot()`



2.8 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

- **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

calc_model(*link*='linear', *B*=None, *lam*=0, *df*=20, *max_itr*=20, *smooth_data*=False, *sparam*=25, *parallel*=False)

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

Parameters

- **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)

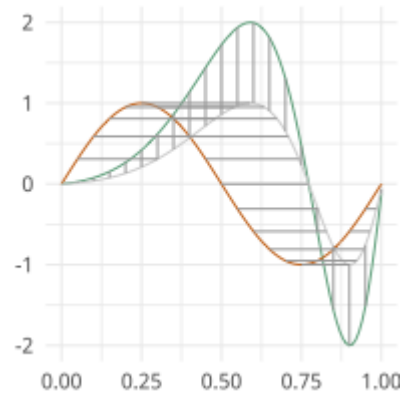
- **sparam** – number of times to apply box filter (default = 25)
- **parallel** – run in parallel (default = F)

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(newdata)`

Parameters

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



2.9 Elastic Functional Tolerance Bounds

Functional Tolerance Bounds using SRSF

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

tolerance.bootTB (*f, time, a=0.05, 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

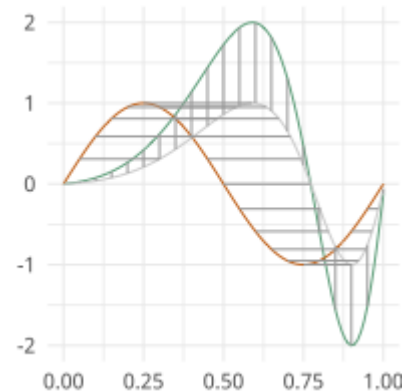
- **df** – degree of freedom
- **p** – number of dimensions

Return type

double

Return R

matrix



2.10 Elastic Functional Clustering

Elastic Functional Clustering

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

`kmeans.kmeans_align(f, time, K, seeds=None, lam=0, showplot=True, smooth_data=False, parallel=False, alignment=True, omethod='DP2', MaxIter=50, thresh=0.01)`

This function clusters functions and aligns using the elastic square-root slope (srsf) framework.

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
- **K** – number of clusters
- **seeds** – indexes of cluster center functions (default = None)
- **lam** – controls the elasticity (default = 0)
- **showplot** – shows plots of functions (default = T)
- **smooth_data** – smooth data using box filter (default = F)

- **parallel** – enable parallel mode using `{link{joblib}}` and `{doParallel}` package (default=F)
- **alignment** – whether to perform alignment (default = T)
- **omethod** – optimization method (DP,DP2,RBFGS)
- **MaxItr** – maximum number of iterations
- **thresh** – cost function threshold

Return type

dictionary

Return fn

aligned functions - matrix (N x M) of M functions with N samples which is a list for each cluster

Return qn

aligned SRSFs - similar structure to fn

Return q0

original SRSFs

Return labels

cluster labels

Return templates

cluster center functions

Return templates_q

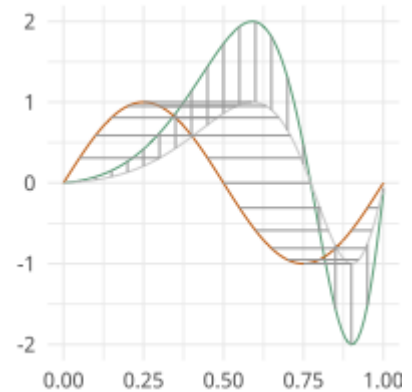
cluster center SRSFs

Return gam

warping functions - similar structure to fn

Return qun

Cost Function



2.11 Elastic Image Warping

image warping using SRVF framework

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

`image.reparam_image(It, Im, gam=None, b=None, stepsize=0.0001, itermax=20)`

This function warps an image to another using SRVF framework

Parameters

- **I_m** – numpy ndarray of shape (N,N) representing a NxN image
- **I_t** – numpy ndarray of shape (N,N) representing a NxN image
- **gam** – numpy ndarray of shape (N,N) representing an initial warping function
- **b** – numpy ndarray representing basis matrix

Return type

numpy ndarray

Return gamnew

diffeomorphism

Return Inew

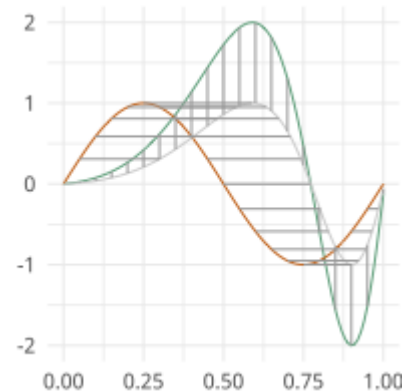
warped image

Return H

energy

Return stepsize

final stepsize



2.12 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 lambda: lambda :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, lam=0.0, 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 = F) :param lam: controls the elasticity (default = 0) :param cores: number of cores for parallel (default = -1 (all)) :param method: method to apply optimization (default="DP") options are "DP" or "RBFSGS"

plot(multivariate=False)

plot curve mean results

Parameters

multivariate – plot as multivariate functions instead of curves (default=False)

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)

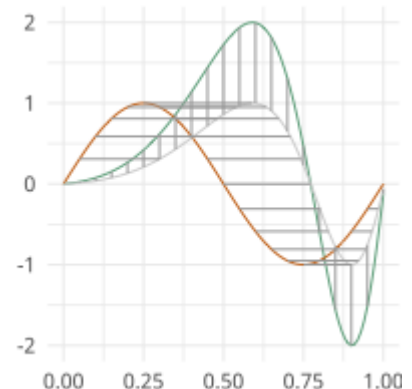
Computes principal direction of variation specified by no. N is Number of shapes away from mean. Creates 2*N+1 shape sequence

Parameters

no – number of direction (default 3)

srvf_align(rotation=True, lam=0.0, 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 lam: controls the elasticity (default = 0) :param parallel: run in parallel (default = F) :param cores: number of cores for parallel (default = -1 (all)) :param method: method to apply optimization (default="DP") options are "DP" or "RBFSGS"



2.13 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)
- **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 geodisc 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, 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
- **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 PsiQ

geodesic path in SRVF

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

Initializes a path in \mathcal{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 \mathcal{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=None, 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 = None, only needed for init “geod”)
- **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.plot_geod(path)`

Plots the geodesic path as a sequence of curves

Parameters

path – numpy ndarray of shape (2,M,K) of M sample points of K samples along path

`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

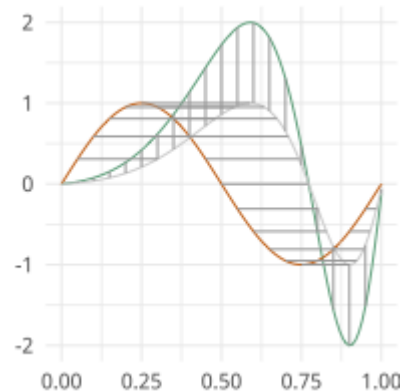
numpy scalar

Return alpha

updated path of srfs

Return beta

updated path of curves



2.14 Utility Functions

Utility functions for SRSF Manipulations

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

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

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))
- **smooth** – smooth warping functions before gradient calculation

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 N warping functions with M 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** – 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

`utility_functions.elastic_depth(f, time, method='DP2', lam=0.0, parallel=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", "cRBFGS"
- **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, alpha=None, return_dt_only=True)`

” 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", "cRBFGS"
- **lam** – controls the elasticity (default = 0.0)
- **alpha** – makes $\alpha * dx + (1-\alpha) * dy$
- **return_dt_only** – returns only dt if alpha is set

Return type

scalar

Return Dy
amplitude distance

Return Dx
phase distance

Return Dt
combined 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 Cmat 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

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='DP2', lam=0.0, penalty='roughness', 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 of second SRSF
- **method** – method to apply optimization (default="DP2") options are "DP", "DP2", "RBFGS", "cRBFGS"
- **lam** – controls the amount of elasticity (default = 0.0)
- **penalty** – penalty type (default="roughness") options are "roughness", "l2gam", "l2psi", "geodesic". Only roughness implemented in all methods. To use others method needs to be "RBFGS" or "cRBFGS"
- **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 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, mu_gam=None)`

Generates random warping functions

Parameters

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

:param mu_gam mean warping function (default identity) :return: 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

- **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.svd_flip(u, v, u_based_decision=True)`

Sign correction to ensure deterministic output from SVD.

Adjusts the columns of u and the rows of v such that the loadings in the columns in u that are largest in absolute value are always positive.

If u_based_decision is False, then the same sign correction is applied to so that the rows in v that are largest in absolute value are always positive.

Parameters

- **u (ndarray)** – Parameters u and v are the output of `linalg.svd` or `randomized_svd()`, with matching inner dimensions so one can compute `np.dot(u * s, v)`.
- **v (ndarray)** – Parameters u and v are the output of `linalg.svd` or `randomized_svd()`, with matching inner dimensions so one can compute `np.dot(u * s, v)`. The input v should really be called vt to be consistent with scipy's output.
- **u_based_decision (bool, default=True)** – If True, use the columns of u as the basis for sign flipping. Otherwise, use the rows of v. The choice of which variable to base the decision on is generally algorithm dependent.

Returns

- **u_adjusted** (*ndarray*) – Array u with adjusted columns and the same dimensions as u.
- **v_adjusted** (*ndarray*) – Array v with adjusted rows and the same dimensions as v.

`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

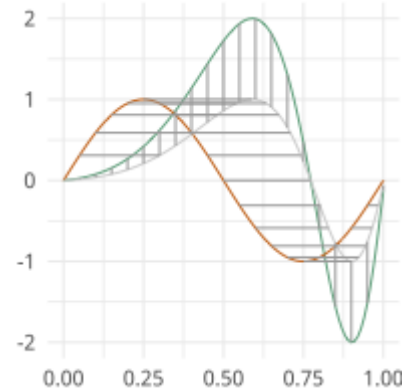
- **Y** – response
- **q** – predictive function
- **bt** – basis function
- **time** – time samples
- **y_max** – maximum response for warping function gmax
- **y_min** – minimum response for warping function gmin
- **gmax** – max warping function
- **gmin** – min warping function

Return type

numpy array

Return gamma

optimal warping function



2.15 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', scale=True)`

This function converts curve beta to srvf q

Parameters

- **beta** – numpy ndarray of shape (2,M) of M samples
- **mode** – Open ('O') or closed curve ('C') (default 'O')
- **scale** – scale curve to unit length (default = True)

Return type

numpy ndarray

Return q

srvf of curve

Return lenb

length of curve

Return lenq

length of srvf

`curve_functions.curve_zero_crossing(Y, q, bt, 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 curve regression model**Parameters**

- **Y** – response
- **beta** – predicitive 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 fuction

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 in R^M : param beta1: numpy ndarray of shape (M,N) of N samples :param beta2: numpy ndarray of shape (M,N) of N 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, lam=0.0, 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)
- **lam** – controls the elasticity (default = 0)
- **method** – method to apply optimization (default="DP") options are "DP" or "RBFSGS"

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, 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

`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 of second SRVF
- **lam** – controls the amount of elasticity (default = 0.0)

- **method** – method to apply optimization (default="DP") options are "DP" or "RBFSGS"

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, 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

`curve_functions.shift_f(f, tau)`

shifts a curve f by tau

Parameters

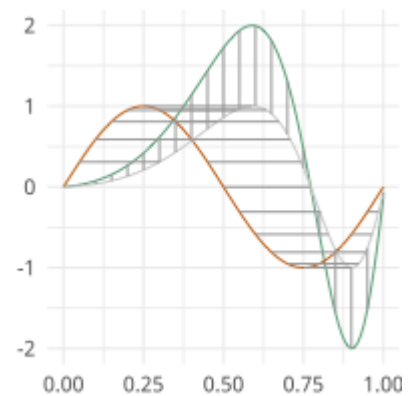
- **f** – numpy ndarray of shape (2,M) of M samples
- **tau** – scalar

Return type

numpy ndarray

Return fn

shifted curve



2.16 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, alpha=0)`

” 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
- **alpha** – weight between phase and amplitude (default = 0, returns amplitude)

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

INSTALLATION

Currently, *fdasrsf* is available in Python versions above 3.8, regardless of the platform. The stable version can be installed via [PyPI](#):

```
pip install fdasrsf
```

It is also available from conda-forge:

```
conda install -c conda-forge fdasrsf
```

It is possible to install the latest version of the package, available in the develop branch, by cloning this repository and doing a manual installation.

```
git clone https://github.com/jdtuck/fdasrsf_python.git
pip install ./fdasrsf_python
```

In this type of installation make sure that your default Python version is currently supported, or change the python and pip commands by specifying a version, such as python3.8.

HOW DO I START?

If you want a quick overview of the package, we recommend you to look at the example notebooks in the *[Users Guide](#)*

CONTRIBUTIONS

All contributions are welcome. You can help this project grow in multiple ways, from creating an issue, reporting an improvement or a bug, to doing a repository fork and creating a pull request to the development branch.

LICENSE

The package is licensed under the BSD 3-Clause License. A copy of the [license](#) can be found along with the code or in the project page.

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