# fdasrsf Documentation

***Release 2.5.10***

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**Apr 10, 2024**

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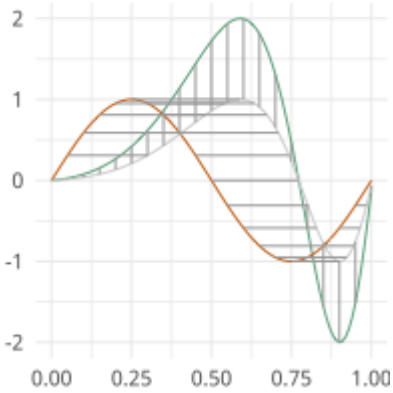
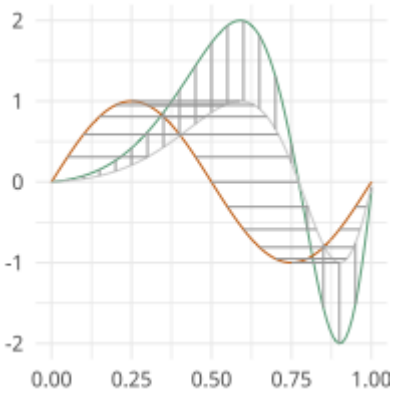



A python package for functional data analysis using the square root slope framework and curves using the square root velocity framework which performs pair-wise and group-wise alignment as well as modeling using functional component analysis and regression.

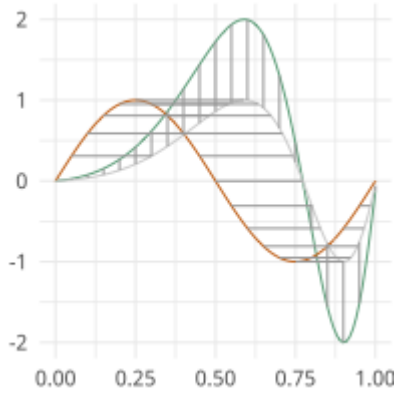


CHAPTER

# ONE

# USER GUIDE

Contents:




## 1.1 Elastic Functional Alignment

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

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

Load in our example data

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

We will then construct the `fdawarp` object

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

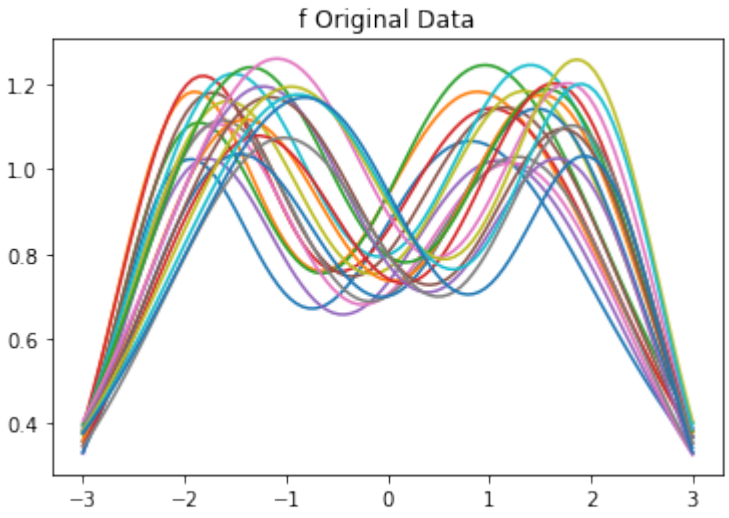
Next we will align the functions using the elastic framework

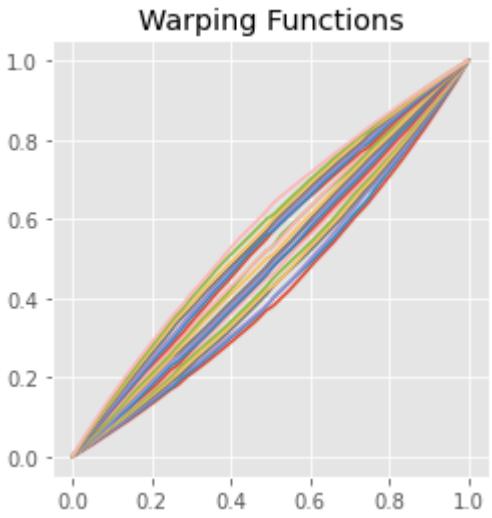
[4]:
```
obj.srsf_align(parallel=True)
```

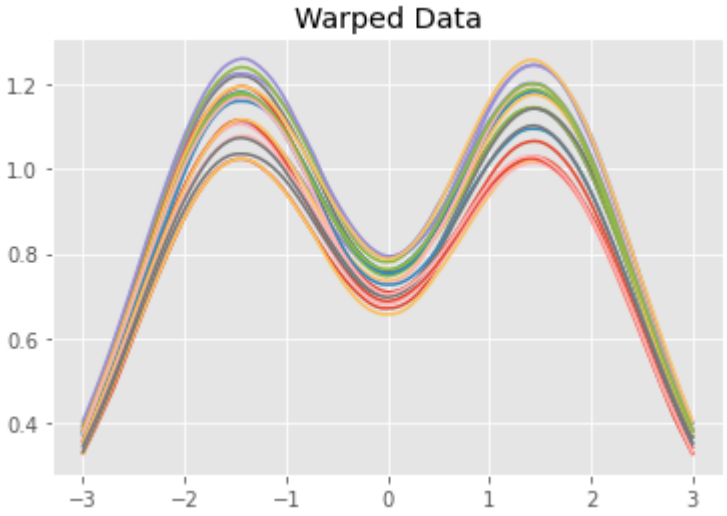
```
Initializing...
Compute Karcher Mean of 21 function in SRSF space...
updating step: r=1
updating step: r=2
```

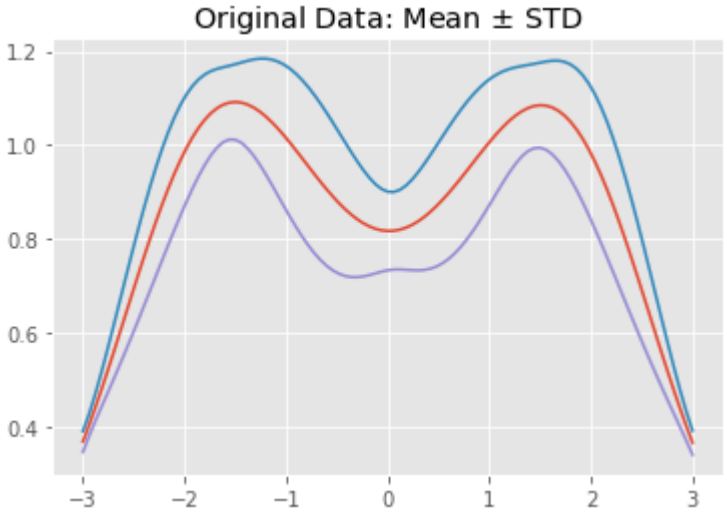
Display plots demonstrating the alignment

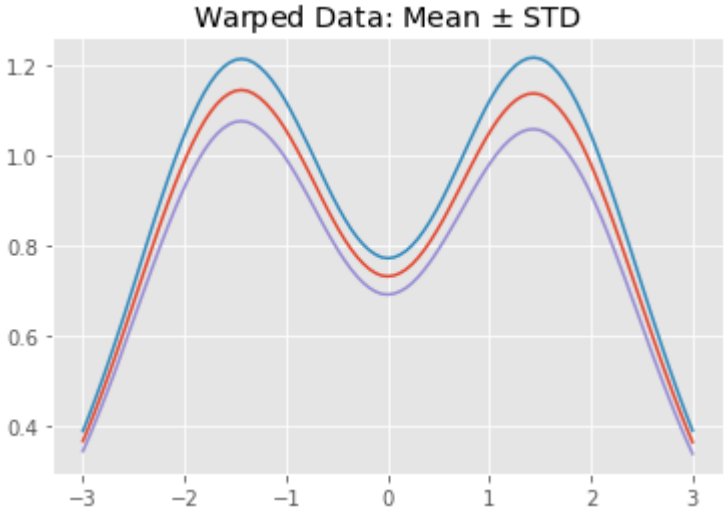
[5]:
```
obj.plot()
```

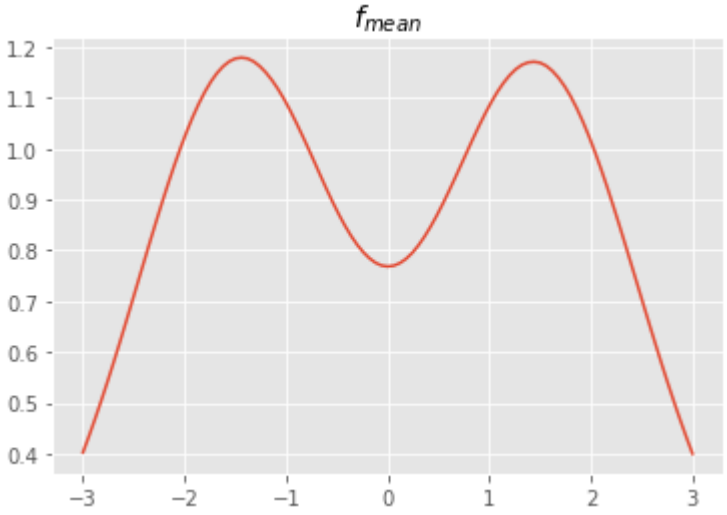


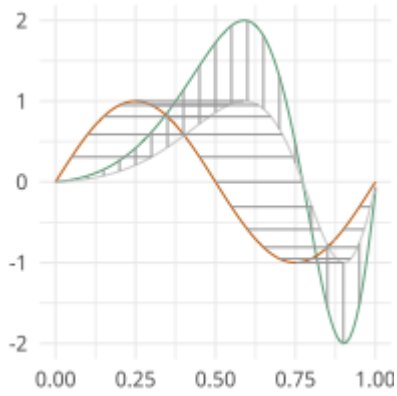




Warped Data
1.2
1.0
0.8
0.6
0.4
−3
−2
−1
0
1
2
3


Original Data: Mean ± STD
1.2
1.0
0.8
0.6
0.4
−3
−2
−1
0
1
2
3


Warped Data: Mean ± STD
1.2
1.0
0.8
0.6
0.4
−3
−2
−1
0
1
2
3




## 1.2 Elastic Functional Principal Component Analysis

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

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

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

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

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

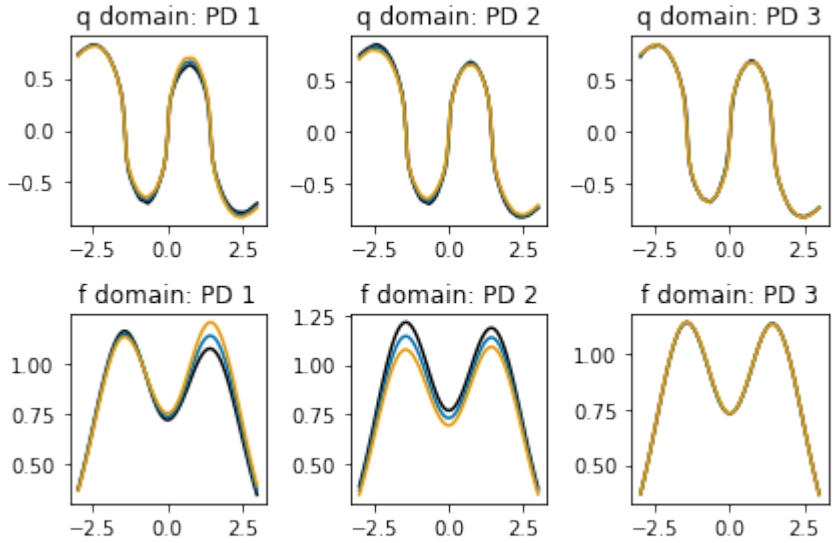
### 1.2.1 Vertical fPCA

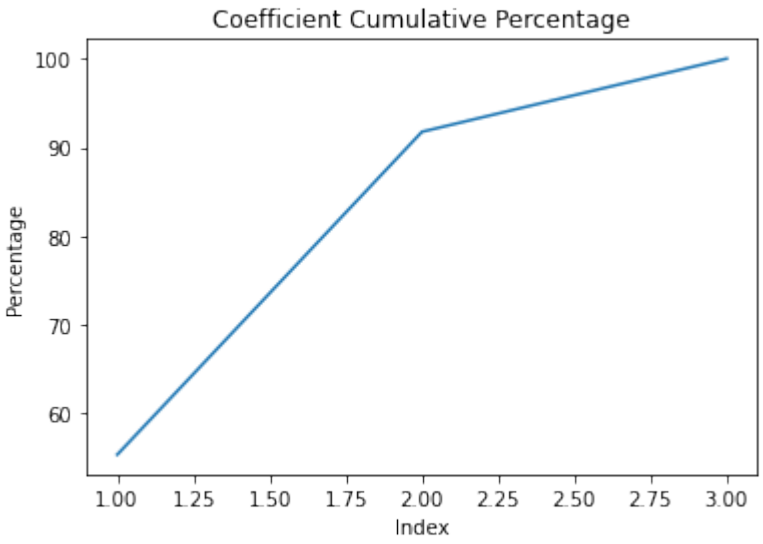
We will first compute fPCA on the aligned functions, by constructing the object and computing the PCA for the number of components, default=3)

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

We then can plot the principal directions

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



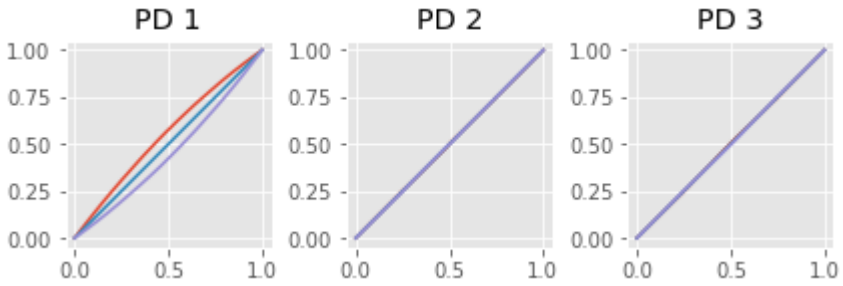
### 1.2.2 Horizontal fPCA

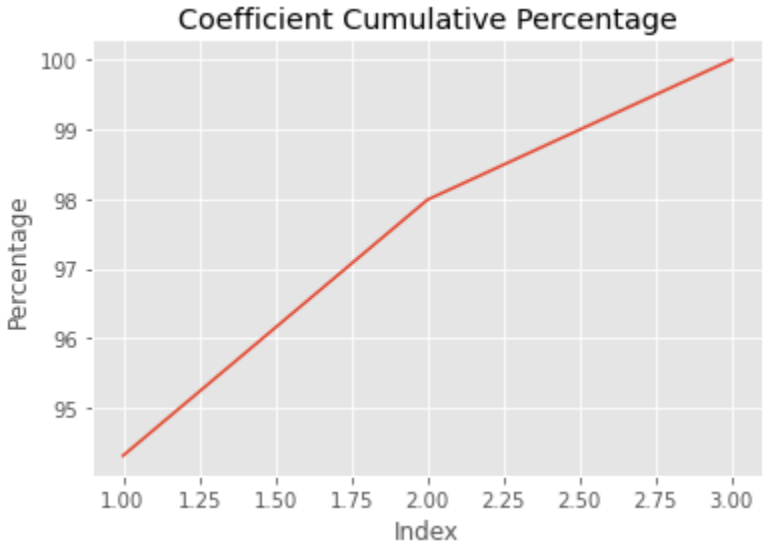
We can then compute PCA on the set of warping functions

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

We then can plot the principal directions

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



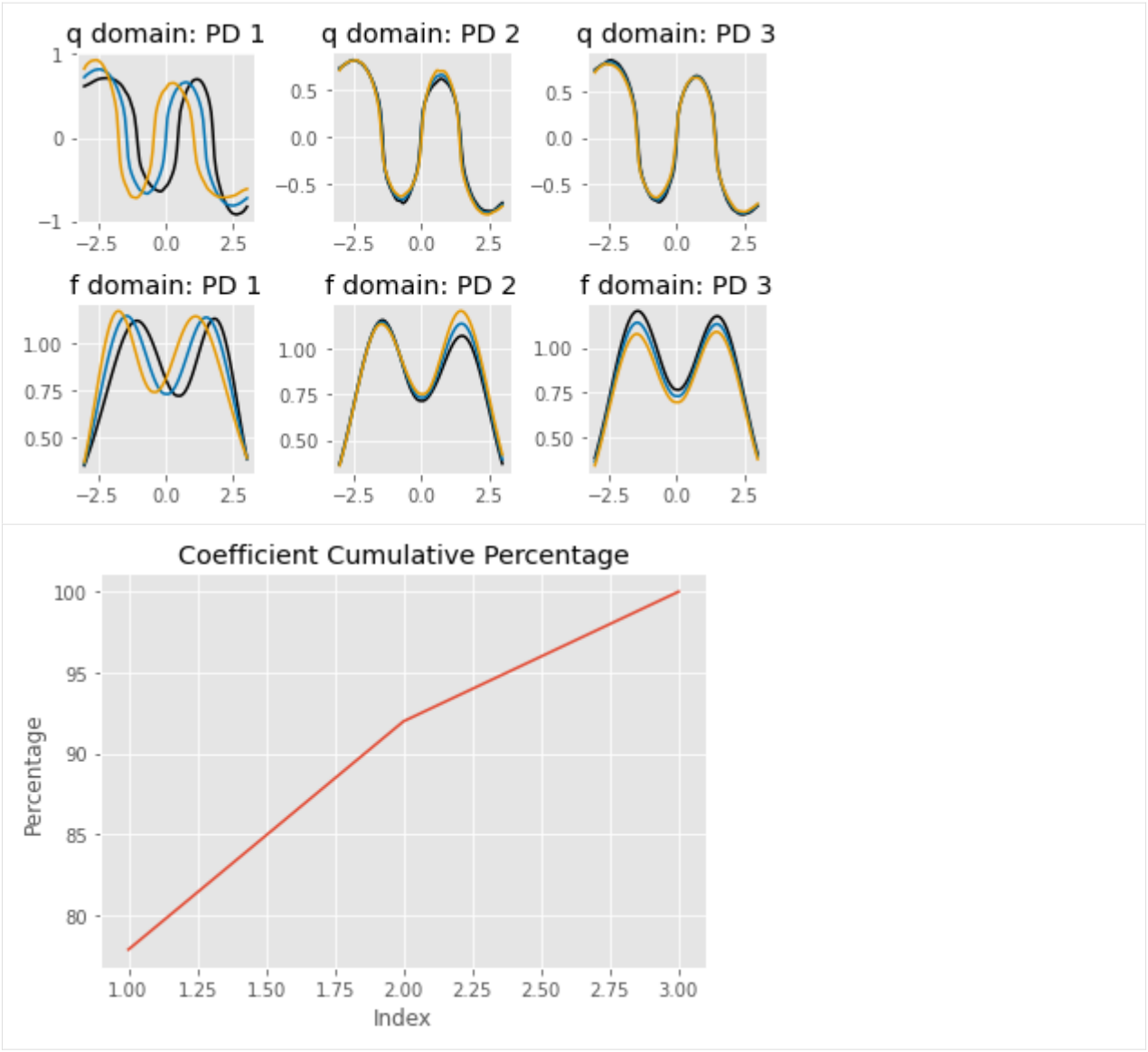

### 1.2.3 Joint fPCA

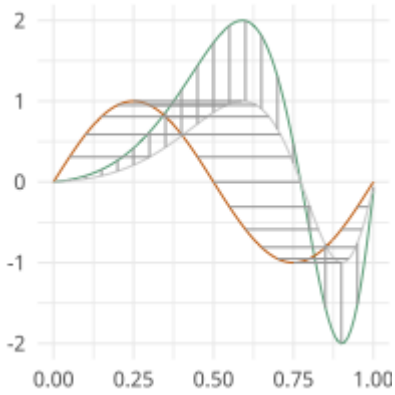
We can also compute the fPCA on jointly on the phase/amplitude space if we feel there is correlation between the variabilities

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

We then can plot the principal directions

[8]:
```
jpca.plot()
```


q domain: PD 1
q domain: PD 2
q domain: PD 3
f domain: PD 1
f domain: PD 2
f domain: PD 3
Coefficient Cumulative Percentage
Percentage
Index



## 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)
```

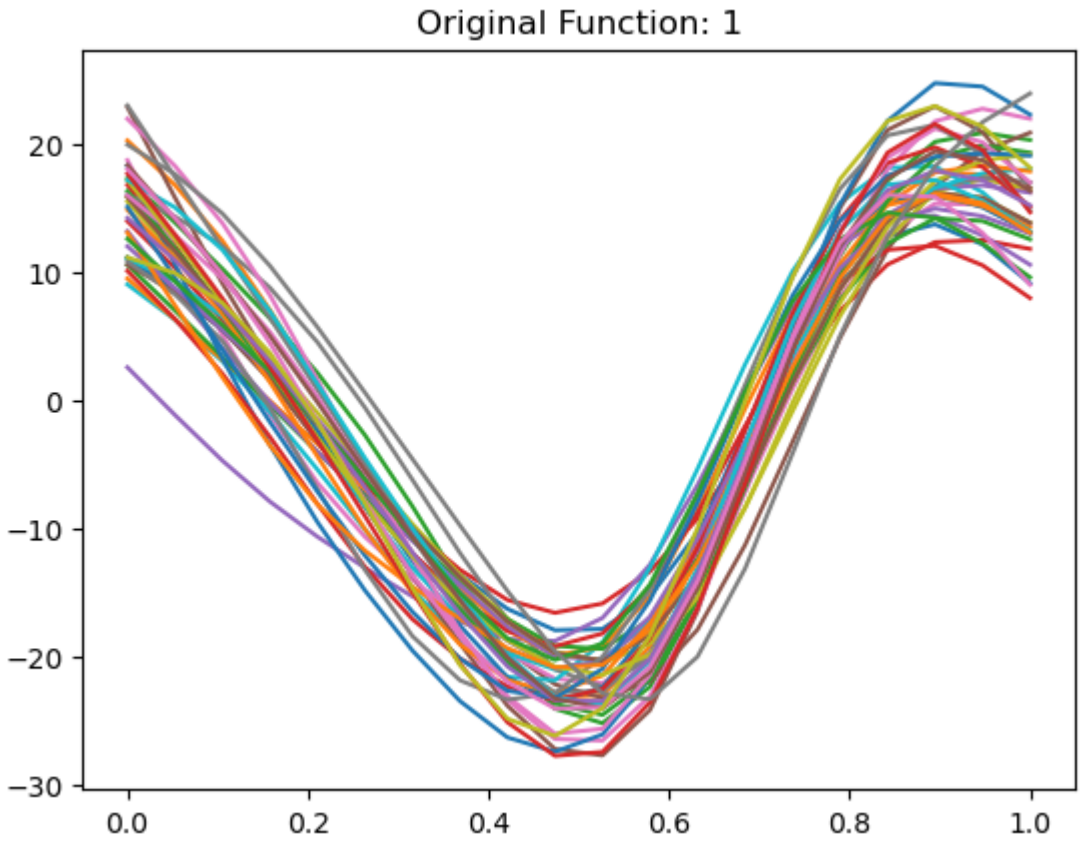
Next, find the Karcher mean and align the curves to the mean

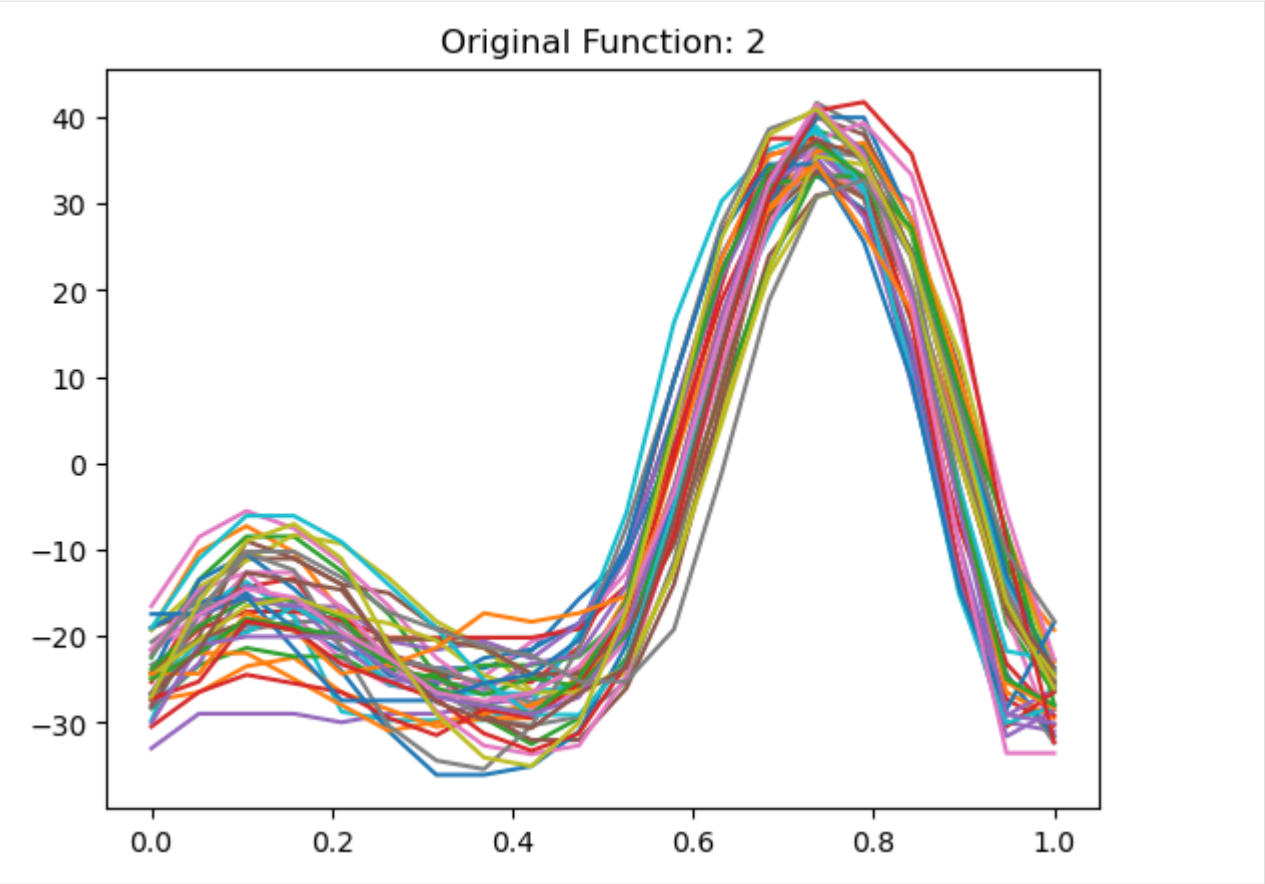
[ ]:
```
obj.karcher_mean(rotation=False)
obj.srvf_align(rotation=False)
```

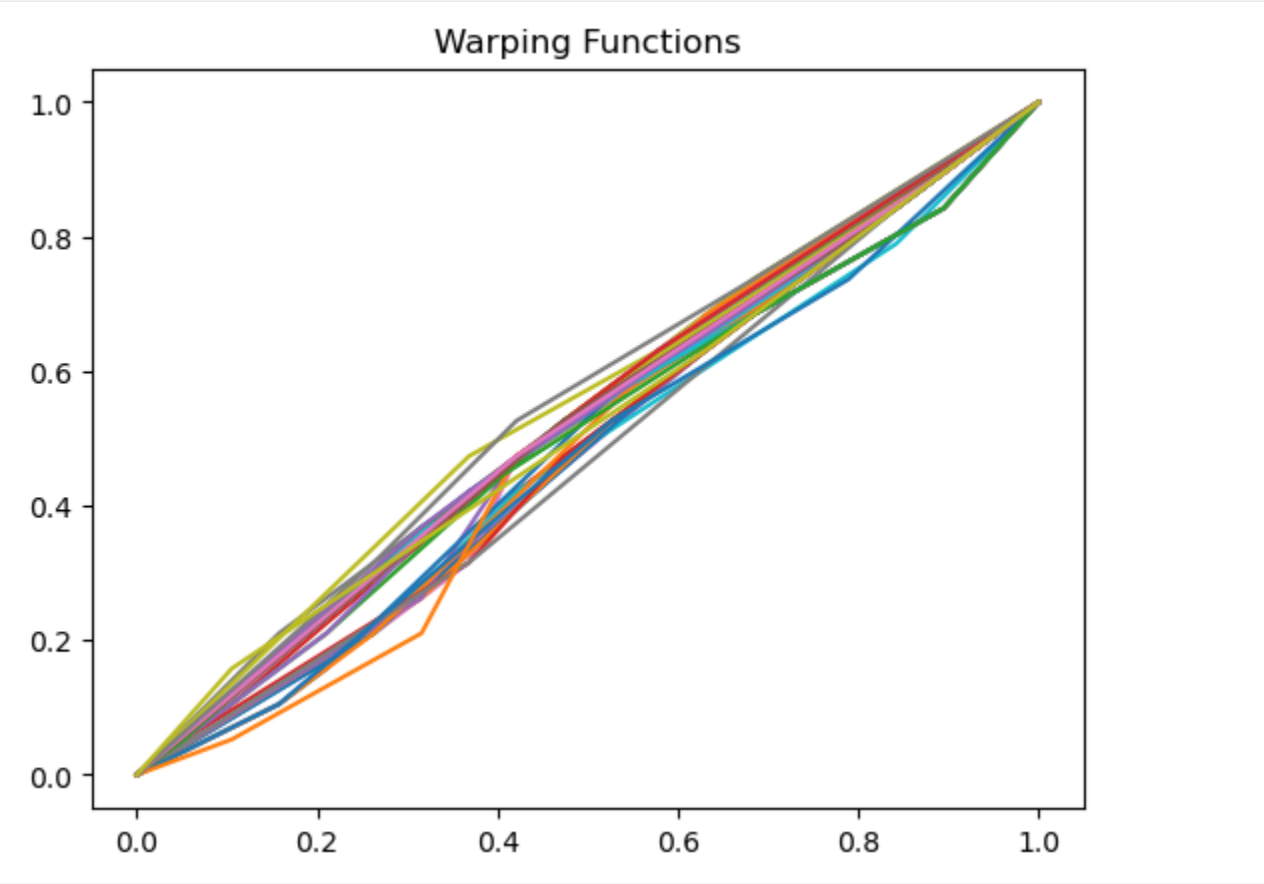
```
Computing Karcher Mean of 39 curves in SRVF space with lam=0
updating step: 1
updating step: 2
updating step: 3
updating step: 4
updating step: 5
updating step: 6
updating step: 7
updating step: 8
updating step: 9
updating step: 10
updating step: 11
```

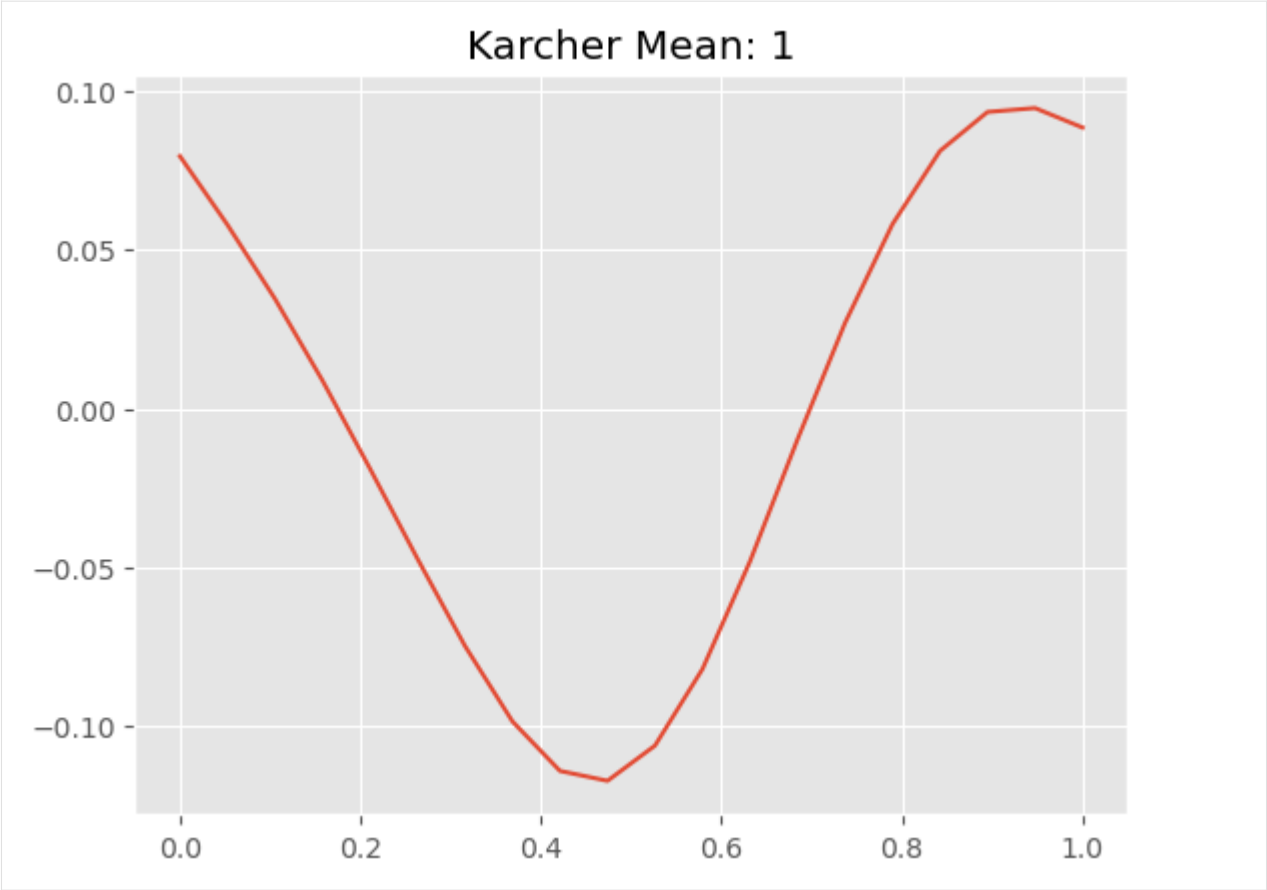
We will now plot the results

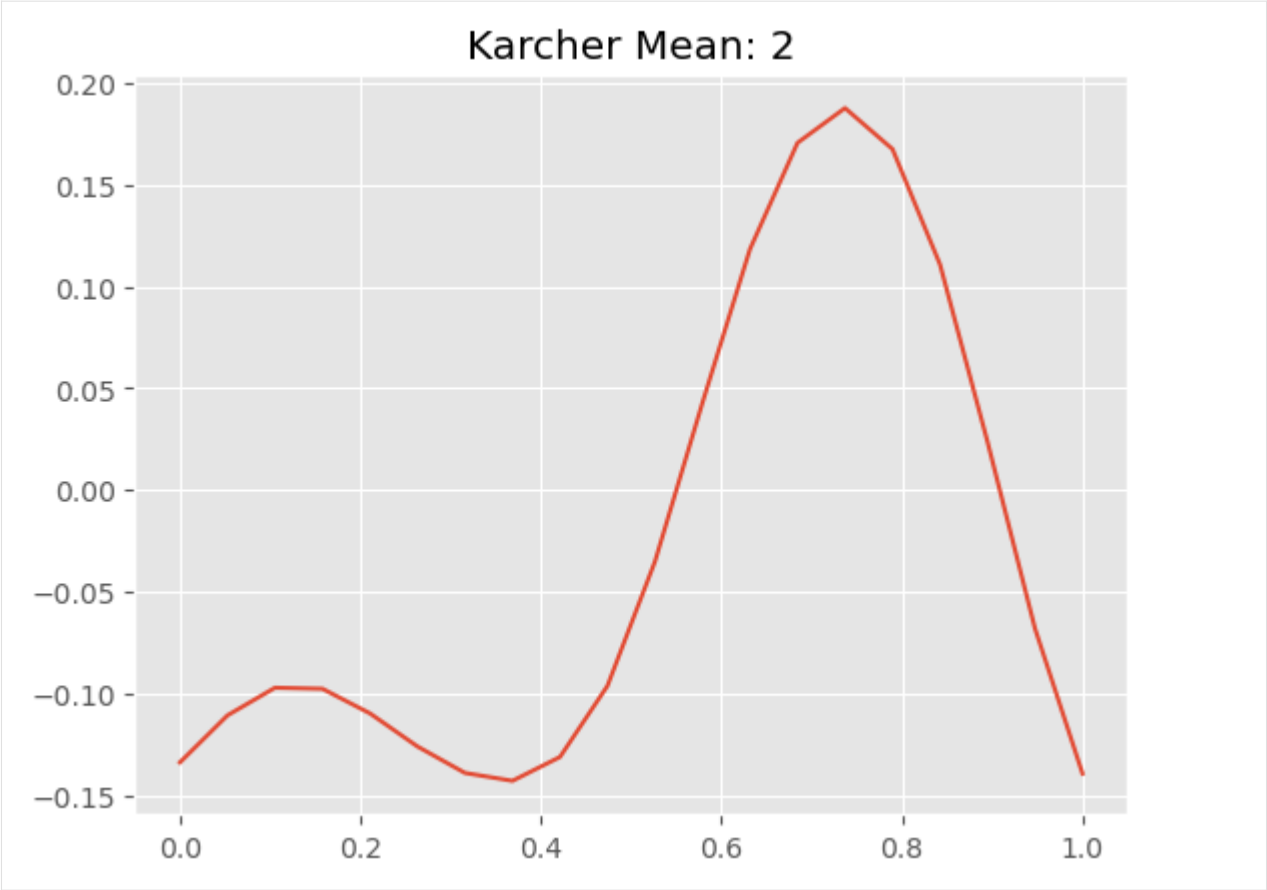
[ ]:
```
obj.plot(multivariate=True)
```

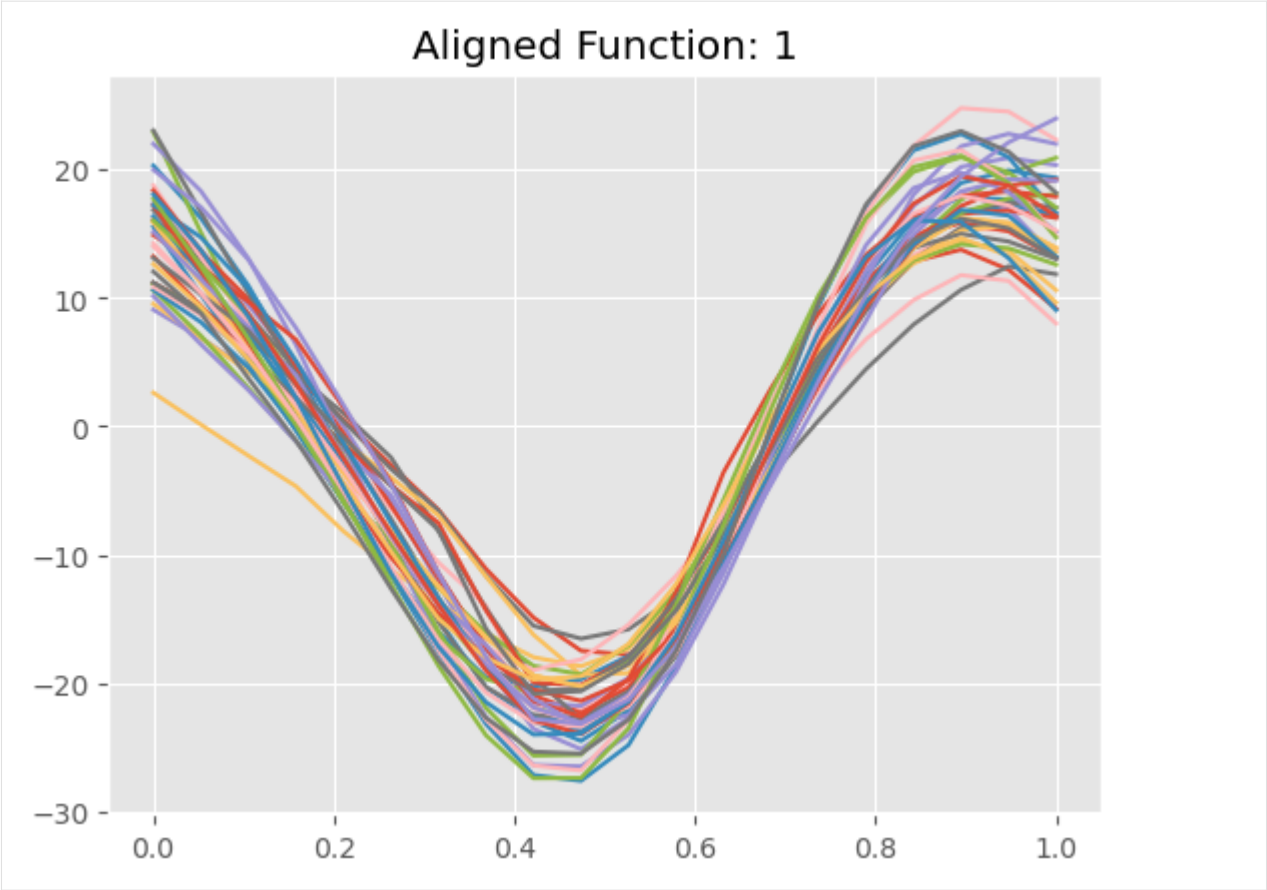


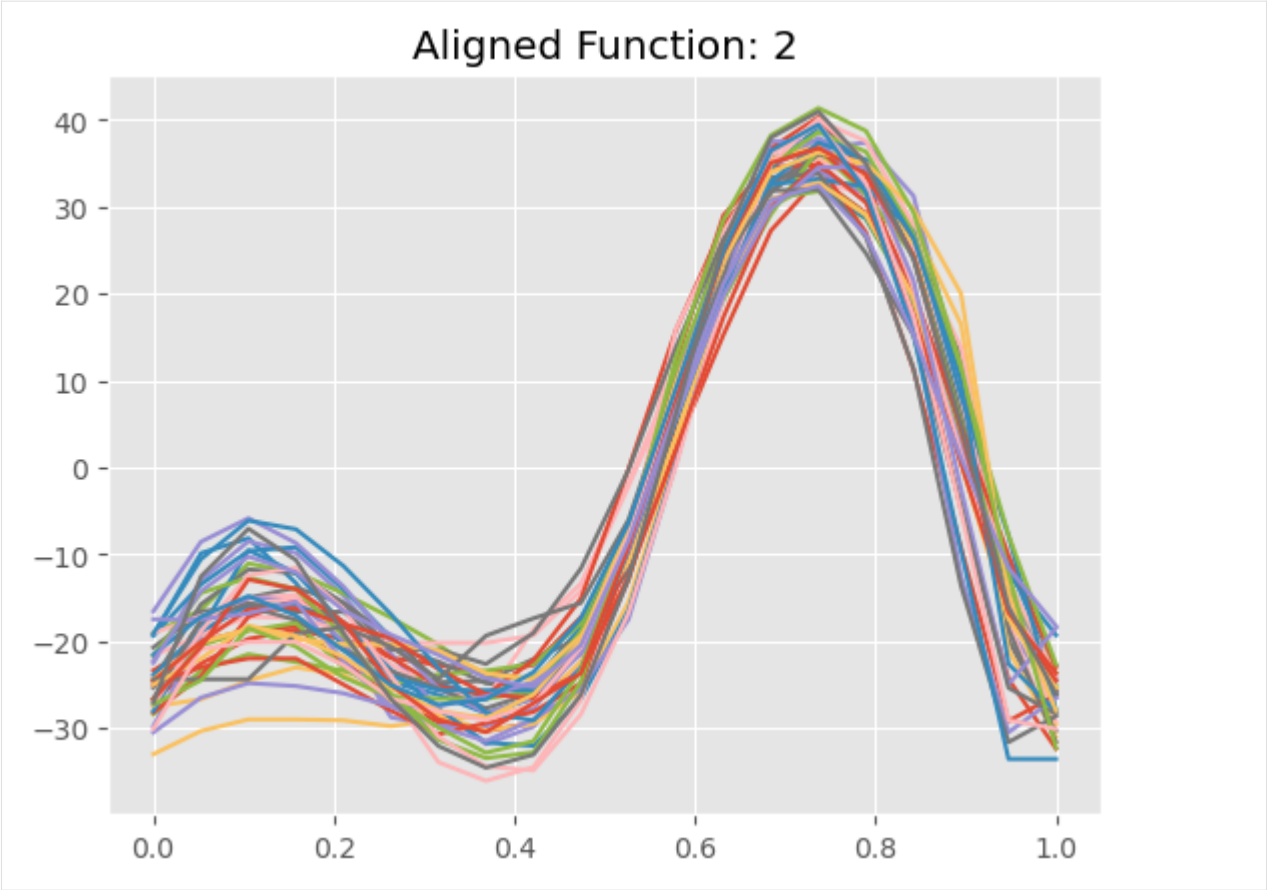

Original Function: 2
40
30
20
10
0
−10
−20
−30
0.0
0.2
0.4
0.6
0.8
1.0


Warping Functions
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0

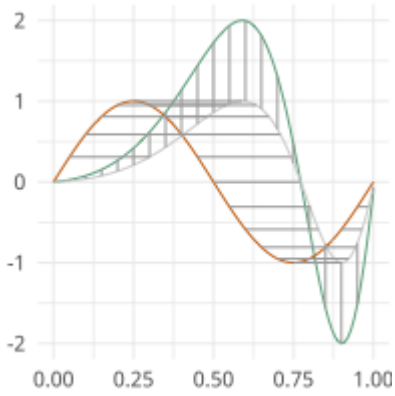

Karcher Mean: 1
0.10
0.05
0.00
−0.05
−0.10
0.0
0.2
0.4
0.6
0.8
1.0


Karcher Mean: 2
0.20
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
0.0
0.2
0.4
0.6
0.8
1.0


Aligned Function: 1
20
10
0
−10
−20
−30
0.0
0.2
0.4
0.6
0.8
1.0


Aligned Function: 2
40
30
20
10
0
−10
−20
−30
0.0
0.2
0.4
0.6
0.8
1.0

[ ]:


2
1
0
-1
-2
0.00
0.25
0.50
0.75
1.00

## 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()
```

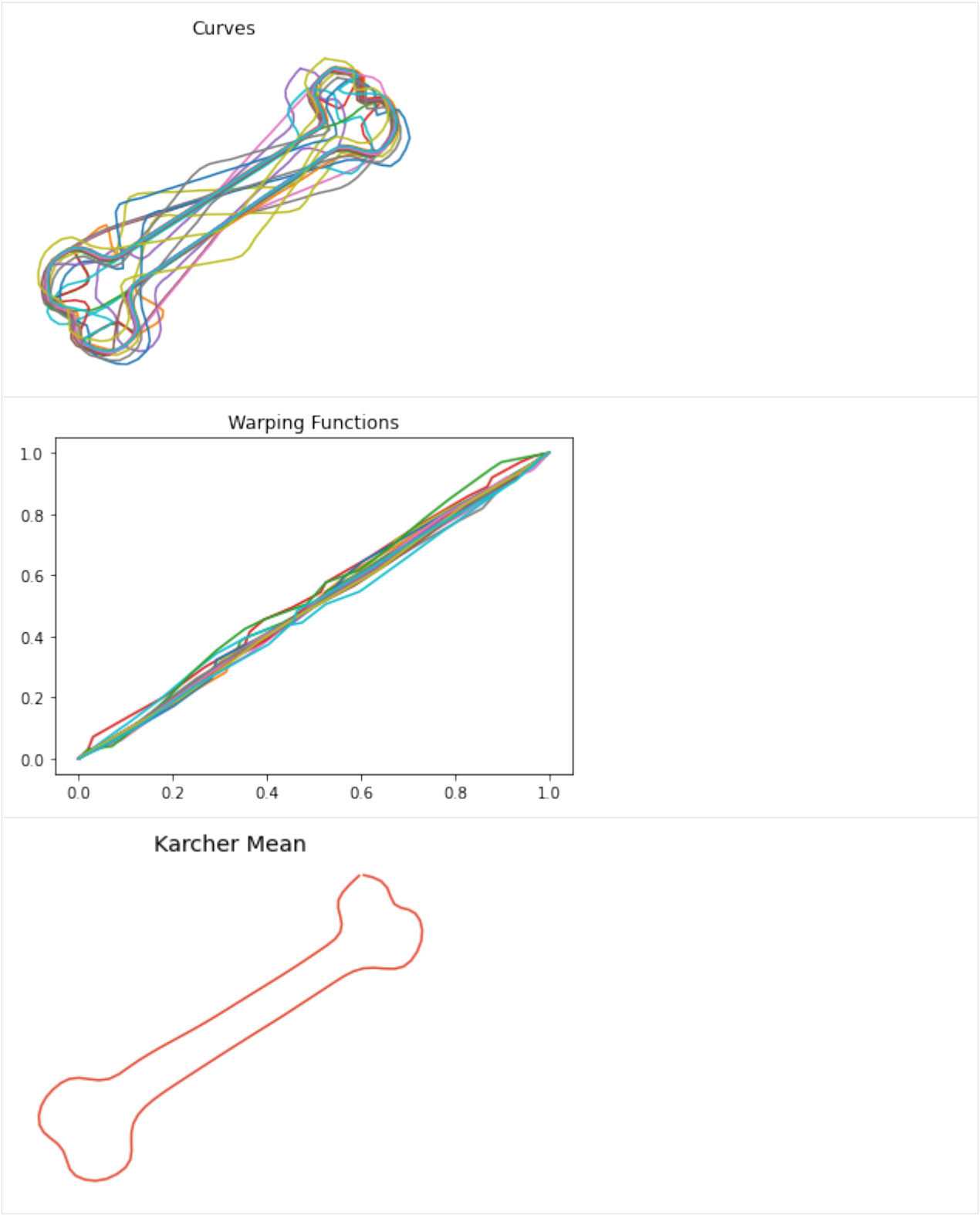
```
Computing Karcher Mean of 20 curves in SRVF space..
updating step: 1
updating step: 2
updating step: 3
updating step: 4
updating step: 5
updating step: 6
updating step: 7
```

We then can align the curves to the karcher mean

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

Plot the results

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


Curves
Warping Functions
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Karcher Mean

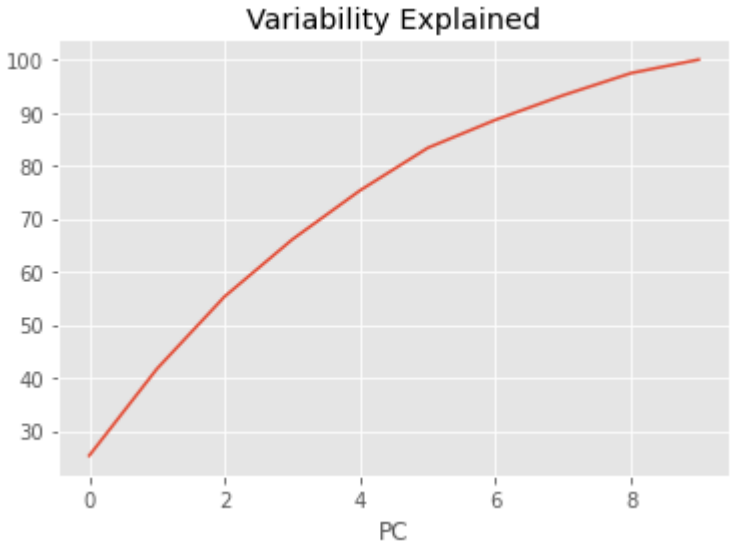
### 1.4.1 Shape PCA

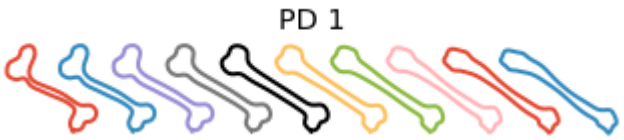
We then can compute the Karcher covariance and compute the shape pca

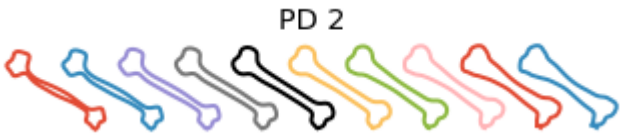
[7]:
```
obj.karcher_cov()
obj.shape_pca()
```

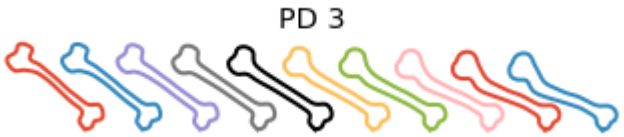
Plot the principal directions

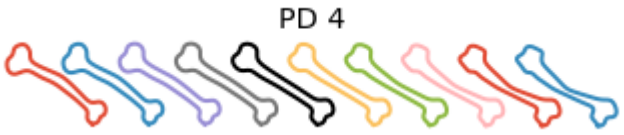
[8]:
```
obj.plot_pca()
```

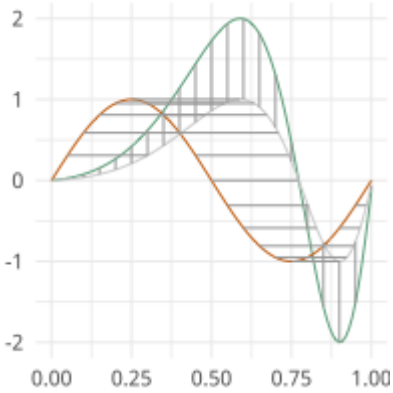


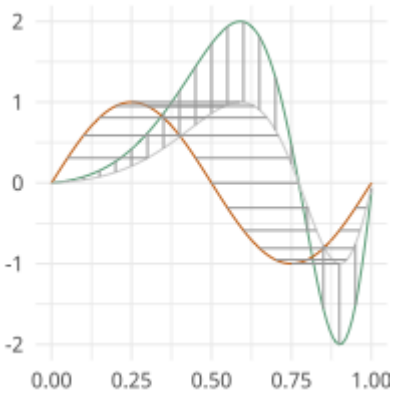




2
1
0
-1
-2
0.00
0.25
0.50
0.75
1.00

CHAPTER

TWO

# 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*, *MaxItr=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, RBFGS, cRBFGS) (default = DP2)
- **center** – center warping functions (default = T)
- **smoothdata** (*bool*) – Smooth the data using a box filter (default = F)
- **MaxItr** – Maximum number of iterations (default = 20)
- **parallel** – run in parallel (default = F)
- **lam** (*double*) – controls the elasticity (default = 0)
- **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)
- **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.**normal**(*loc=0.0*, *scale=1.0*, *size=None*)

Draw random samples from a normal (Gaussian) distribution.

The probability density function of the normal distribution, first derived by De Moivre and 200 years later by both Gauss and Laplace independently[2], is often called the bell curve because of its characteristic shape (see the example below).

The normal distributions occurs often in nature. For example, it describes the commonly occurring distribution of samples influenced by a large number of tiny, random disturbances, each with its own unique distribution[2].

---

**Note:** New code should use the *~numpy.random.Generator.normal* method of a *~numpy.random.Generator* instance instead; please see the random-quick-start.

---

**Parameters**

- **loc** (*float or array_like of floats*) – Mean ("centre") of the distribution.
- **scale** (*float or array_like of floats*) – Standard deviation (spread or "width") of the distribution. Must be non-negative.
- **size** (*int or tuple of ints, optional*) – Output shape. If the given shape is, e.g., `(m, n, k)`, then `m * n * k` samples are drawn. If size is `None` (default), a single value is returned if `loc` and `scale` are both scalars. Otherwise, `np.broadcast(loc, scale).size` samples are drawn.

**Returns**

**out** – Drawn samples from the parameterized normal distribution.

**Return type**

ndarray or scalar

**See also:**

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

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

**random.Generator.normal**
which should be used for new code.

### Notes

The probability density for the Gaussian distribution is

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

where $\mu$ is the mean and $\sigma$ the standard deviation. The square of the standard deviation, $\sigma^2$, is called the variance.

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

### References

### Examples

Draw samples from the distribution:

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

Verify the mean and the variance:

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

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

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

```
>>> import matplotlib.pyplot as plt
>>> count, bins, ignored = plt.hist(s, 30, density=True)
>>> plt.plot(bins, 1/(sigma * np.sqrt(2 * np.pi)) *
...                np.exp( - (bins - mu)**2 / (2 * sigma**2) ),
...          linewidth=2, color='r')
>>> plt.show()
```

Two-by-four array of samples from the normal distribution with mean 3 and standard deviation 2.5:

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

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
- **mcmopts** – dict of mcmc parameters

default mcmc options: tmp = {"betas":np.array([0.5,0.5,0.005,0.0001]),"probs":np.array([0.1,0.1,0.7,0.1])} mcmcopts = {"iter":2*(10**4) ,"burnin":np.minimum(5*(10**3),2*(10**4)//2), "alpha0":0.1, "beta0":0.1,"zpcn":tmp,"propvar":1, "initcoef":np.repeat(0,20), "npoints":200, "extrainfo":True}

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

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

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

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

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

**Parameters**

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

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

Basis can be 'fourier' or 'legendre'

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

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

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

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

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

Random values in a given shape.

---

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

---

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

**Parameters**

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

**Returns**
**out** – Random values.

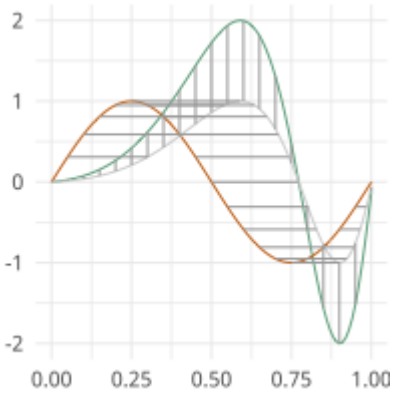
**Return type**
ndarray, shape `(d0, d1, ..., dn)`

**See also:**

random

### Examples

```
>>> np.random.rand(3,2)
array([[ 0.14022471,  0.96360618],  #random
       [ 0.37601032,  0.25528411],  #random
       [ 0.49313049,  0.94909878]]) #random
```




## 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*)

This function calculates joint functional principal component analysis on aligned data

**Parameters**

- **var_exp** – compute no based on value percent variance explained (default: 0.99)
- **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()

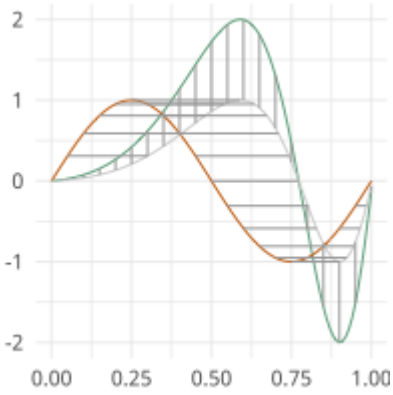
**project**(*f*)

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.

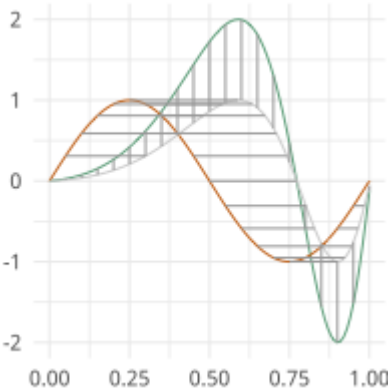
**Parameters**

- **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)

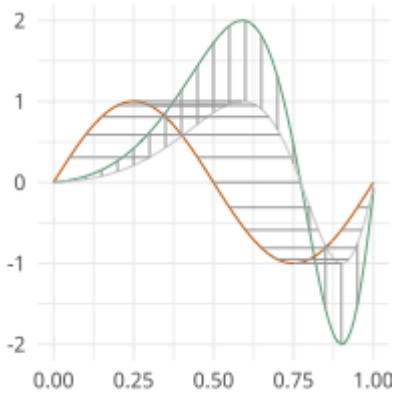
**Return type**
numpy ndarray

**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 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*)

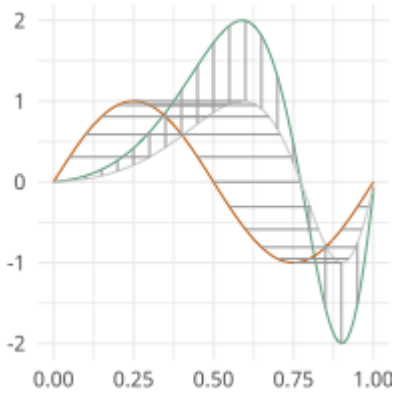
calculates optimal warping for function linear regression

**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**

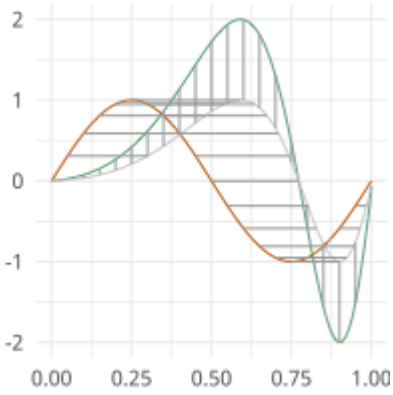
- **pca_method** – string specifying pca method (options = "combined", "vert", or "horiz", default = "combined")
- **no** – scalar specify number of principal components (default=5)
- **var_exp** – compute no based on value percent variance explained (example: 0.95)
- **smooth_data** – smooth data using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

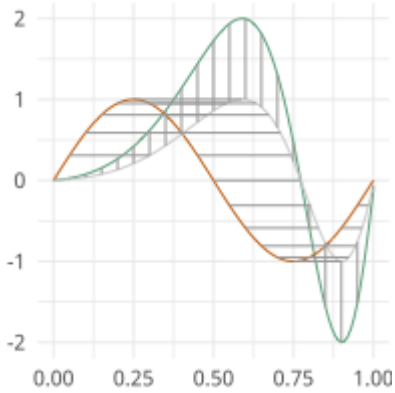
**compute**(*d=1000*, *h=0*, *M_approx=365*)

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

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

Random values in a given shape.

---

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

---

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

**Parameters**

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

**Returns**

**out** – Random values.

**Return type**

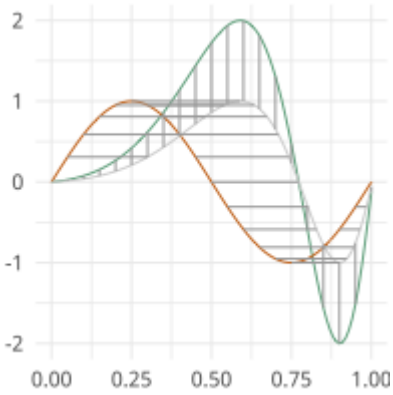
ndarray, shape `(d0, d1, ..., dn)`

**See also:**

`random`

### Examples

```
>>> np.random.rand(3,2)
array([[ 0.14022471,  0.96360618],  #random
       [ 0.37601032,  0.25528411],  #random
       [ 0.49313049,  0.94909878]]) #random
```




## 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*)

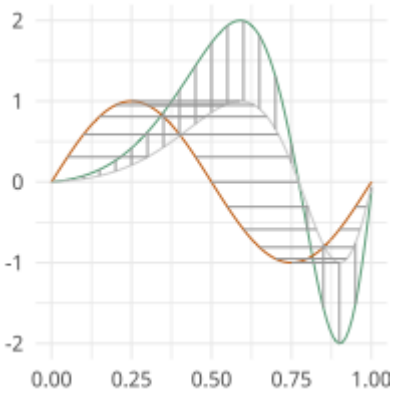
Computes a random wishart matrix

**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'*, *MaxItr=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 code{link{joblib}} and code{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

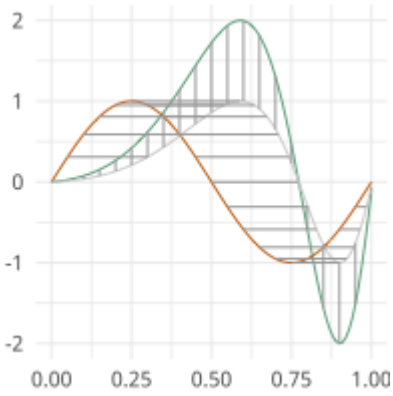
**Return labels**
cluster labels

**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**

- **Im** – numpy ndarray of shape (N,N) representing a NxN image
- **Im** – 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

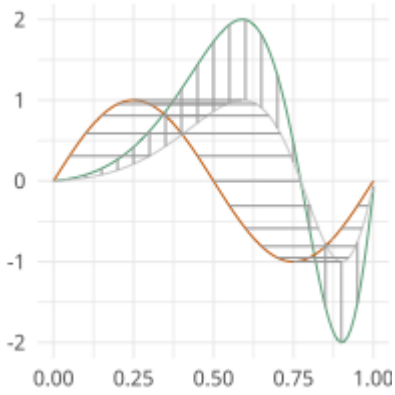
**Return type**
numpy ndarray

**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 "RBFGS"

**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 "RBFGS"

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

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

---

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

---

---

**Note:** New code should use the *~numpy.random.Generator.standard_normal* method of a *~numpy.random.Generator* instance instead; please see the random-quick-start.

---

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

**Parameters**

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

**Returns**

**Z** – A `(d0, d1, ..., dn)`-shaped array of floating-point samples from the standard normal distribution, or a single such float if no parameters were supplied.

**Return type**

ndarray or float

**See also:**

`standard_normal`
Similar, but takes a tuple as its argument.

`normal`
Also accepts mu and sigma arguments.

`random.Generator.standard_normal`
which should be used for new code.

### Notes

For random samples from the normal distribution with mean `mu` and standard deviation `sigma`, use:

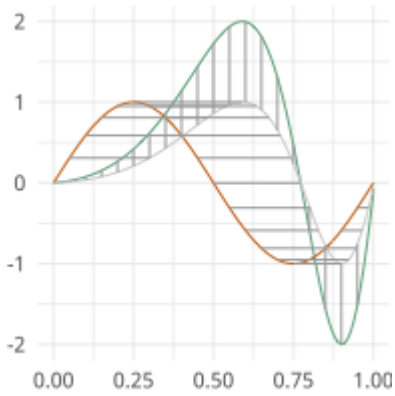
```
sigma * np.random.randn(...) + mu
```

### Examples

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

Two-by-four array of samples from the normal distribution with mean 3 and standard deviation 2.5:

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



## 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

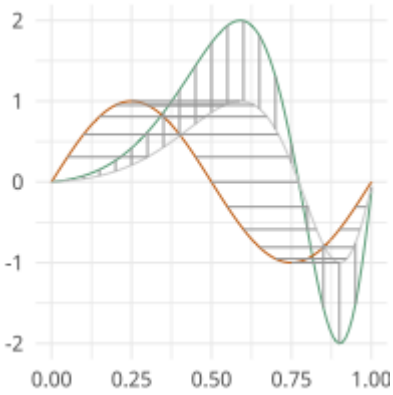
**Parameters**

- **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 paramenter
- **T** – Number of samples of curve (Default = 100)
- **k** – number of samples along path (Default = 5)

**Return type**
numpy scalar

**Return alpha**
updated path of srvfs

**Return beta**
updated path of curves




## 2.14 Utility Functions

Utility functions for SRSF Manipulations

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

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

calculates the srsf of warping functions with corresponding shooting vectors

**Parameters**

- **gam** – numpy ndarray of shape (M,N) of M warping functions with N samples
- **parallel** – run in parallel (default = F)
- **cores** – number of cores for parallel (default = -1 (all))

**Return type**
2 numpy ndarray and vector

**Return mu**
Karcher mean psi function

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

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

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

utility_functions.**SqrtMeanInverse**(*gam*)

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

**Parameters**
**gam** – numpy ndarray of shape (M,N) of 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 tr L'AM / sqrt(tr L'BL tr M'CM) w.r.t. L and M

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

**Return type**
numpy ndarray

**Return values**
eigenvalues

**Return Lmat**
left eigenvectors

**Return Mmat**
right eigenvectors

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

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

**Parameters**

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

**Return type**
tuple of numpy ndarray

**Return f0**
smoothed functions functions

**Return g**
first derivative of each function

**Return g2**
second derivative of each function

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

calculates the innerproduct between two srsfs

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

**Return type**
scalar

**Return val**
inner product value

utility_functions.**invertGamma**(*gam*)

finds the inverse of the diffeomorphism gamma

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

**Return type**
vector

**Return gamI**
inverse of gam

utility_functions.**optimum_reparam**(*q1*, *time*, *q2*, *method='DP2'*, *lam=0.0*, *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 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 samples of second SRSF
- **q2** – vector of size N or array of NxM samples samples of second SRSF
- **lam** – controls the amount of elasticity (default = 0.0)

**Return type**
vector

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

utility_functions.**outlier_detection**(*q*, *time*, *mq*, *k=1.5*)

calculates outlier's using geodesic distances of the SRSFs from the median

**Parameters**

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

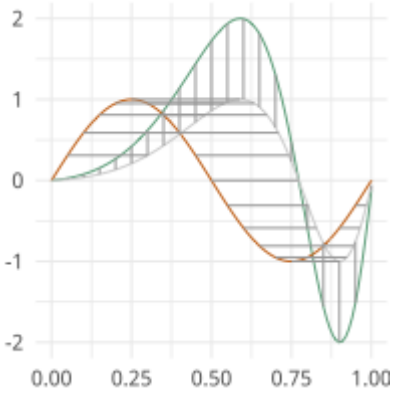
finds zero-crossing of optimal gamma, gam = s*gmax + (1-s)*gmin from elastic regression model

**Parameters**

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

**Return type**
numpy array

**Return gamma**
optimal warping function




## 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'*)

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')

**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, gam = s*gmax + (1-s)*gmin from elastic curve regression model

**Parameters**

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

**Return type**
numpy array

**Return gamma**
optimal warping function

**Return O_hat**
rotation matrix

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

Calculates the two elastic distances between two curves 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 "RBFGS"

**Return type**
numpy ndarray

**Return beta2new**
optimal rotated beta2 to beta1

**Return O**
rotation matrix

**Return tau**
seed

curve_functions.**gram_schmidt**(*basis*)

Performs Gram Schmidt Orthogonlization of a basis_o

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

**rtype**
list of numpy ndarray

**return basis_o**
orthogonlized basis

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

This function reparamerized srvf q by gamma

**Parameters**

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

**Return type**
numpy ndarray

**Return qn**
reparatermized srvf

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

This function reparamerized curve f by gamma

**Parameters**

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

**Return type**
numpy ndarray

**Return fn**
reparatermized curve

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

This function calculates the inner product in srvf space

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

**Return type**
vector

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

curve_functions.**parallel_translate**(*w*, *q1*, *q2*, *basis*, *mode=0*)

parallel translates q1 and q2 along manifold

**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 prepcoessed 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*)

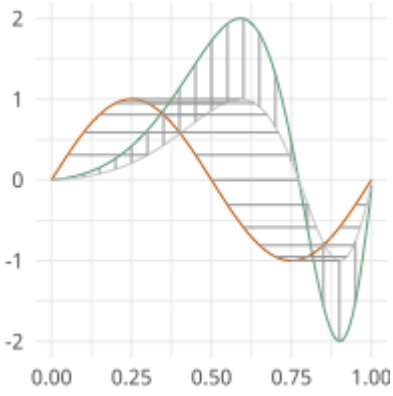
shifts a curve f by tau

**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

CHAPTER

THREE

# 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.

CHAPTER

FOUR

# 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*

CHAPTER

FIVE

# 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.

CHAPTER

SIX

# 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.

CHAPTER

# SEVEN

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EIGHT

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