# **fdasrsf Documentation**

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

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## **FUNCTIONAL ALIGNMENT**

Group-wise function alignment using SRSF framework and Dynamic Programming

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

time\_warping.align\_fPCA (f, time, num\_comp=3, showplot=True, smoothdata=False) aligns a collection of functions while extracting principal components. The functions are aligned to the principal components

## **Parameters**

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

**Return type** tuple of numpy array

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

Return qn aligned srvfs - similar structure to fn

Return q0 original srvf - similar structure to fn

Return mqn srvf mean or median - vector of length M

Return gam warping functions - similar structure to fn

Return q\_pca srsf principal directions

Return f\_pca functional principal directions

Return latent latent values

Return coef coefficients

Return U eigenvectors

Return orig\_var Original Variance of Functions

Return amp\_var Amplitude Variance

Return phase\_var Phase Variance

time\_warping.align\_fPLS(f, g, time, comps=3, showplot=True, smoothdata=False, delta=0.01, max itr=100)

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

## **Parameters**

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

**Return type** tuple of numpy array

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

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

 $time\_warping. \textbf{srsf\_align} (\textit{f}, time, method='mean', omethod='DP', showplot=True, smooth-\\ data=False, parallel=False, lam=0.0)$ 

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

## **Parameters**

- $\mathbf{f}$  numpy ndarray of shape (M,N) of N functions with M samples
- time vector of size M describing the sample points
- method (string) warp calculate Karcher Mean or Median

(options = "mean" or "median") (default="mean") :param omethod: optimization method (DP, DP2, RBFGS) (default = DP) :param showplot: Shows plots of results using matplotlib (default = T) :param smoothdata: Smooth the data using a box filter (default = F) :param parallel: run in parallel (default = F) :param lam: controls the elasticity (default = 0) :type lam: double :type smoothdata: bool :type f: np.ndarray :type time: np.ndarray

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 fmean: function mean or median - vector of length M :return mqn: srvf mean or median - vector of length M :return gam: warping functions - similar structure to fn :return orig\_var: Original Variance of Functions :return amp\_var: Amplitude Variance :return phase\_var: Phase Variance

Examples >>> import tables >>> fun=tables.open\_file("../Data/simu\_data.h5") >>> f = fun.root.f[:] >>> f = f.transpose() >>> time = fun.root.time[:] >>> out = srsf\_align(f,time)

time\_warping.srsf\_align\_pair(f, g, time, method='mean', showplot=True, smoothdata=False, lam=0.0)

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

## **Parameters**

• **f** (np.ndarray) – numpy ndarray of shape (M,N) of N functions with M samples

- g numpy ndarray of shape (M,N) of N functions with M samples
- time (np.ndarray) vector of size M describing the sample points
- method (string) warp calculate Karcher Mean or Median (options = "mean" or "median") (default="mean")
- **showplot** Shows plots of results using matplotlib (default = T)
- **smoothdata** (bool) Smooth the data using a box filter (default = F)
- lam (double) controls the elasticity (default = 0)

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 fmean f function mean or median - vector of length N

Return gmean g function mean or median - vector of length N

Return mqfn srvf mean or median - vector of length N

Return mqgn srvf mean or median - vector of length N

Return gam warping functions - similar structure to fn

## FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS

Vertical and Horizontal Functional Principal Component Analysis using SRSF

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

fPCA.horizfPCA(gam, time, no=2, showplot=True)

This function calculates horizontal functional principal component analysis on aligned data

#### **Parameters**

- gam numpy ndarray of shape (M,N) of N warping functions
- time vector of size M describing the sample points
- **no** (int) number of components to extract (default = 2)
- **showplot** (bool) Shows plots of results using matplotlib (default = T)

**Return type** tuple 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

fPCA. jointfPCA (fn, time, qn, q0, gam, no=2, showplot=True)

This function calculates joint functional principal component analysis on aligned data

## **Parameters**

- fn numpy ndarray of shape (M,N) of N aligned functions with M samples
- time vector of size N describing the sample points
- qn numpy ndarray of shape (M,N) of N aligned SRSF with M samples
- **no** (*int*) number of components to extract (default = 2)
- **showplot** (bool) Shows plots of results using matplotlib (default = T)

Return type tuple 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

fPCA.vertfPCA(fn, time, qn, no=2, showplot=True)

This function calculates vertical functional principal component analysis on aligned data

## **Parameters**

- fn numpy ndarray of shape (M,N) of N aligned functions with M samples
- time vector of size N describing the sample points
- qn numpy ndarray of shape (M,N) of N aligned SRSF with M samples
- **no** (*int*) number of components to extract (default = 2)
- **showplot** (bool) Shows plots of results using matplotlib (default = T)

**Return type** tuple 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

## **ELASTIC FUNCTIONAL BOXPLOTS**

**Elastic Functional Boxplots** 

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

boxplots.ampbox (ft, f\_median, qt, q\_median, time, alpha=0.05, k\_a=1)

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

## **Parameters**

- ft numpy ndarray of shape (M,N) of N functions with M samples
- **f\_median** vector of size M describing the median
- qt numpy ndarray of shape (M,N) of N srsf functions with M samples
- q\_median vector of size M describing the srsf median
- time vector of size M describing the time
- alpha quantile value (e.g.,=.05, i.e., 95%)
- **k a** scalar for outlier cutoff (e.g.,=1)

**Return type** tuple of numpy array

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

functions with M samples :return Q1: First quartile :return Q3: Second quartile :return Q1a: First quantile based on alpha :return Q3a: Second quantile based on alpha :return minn: minimum extreme function :return maxx: maximum extreme function :return outlier\_index: indexes of outlier functions :return f\_median: median function :return q median: median srsf :return plt: surface plot mesh

boxplots.phbox (gam, time, alpha=0.05,  $k_a=1$ )

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

## **Parameters**

- gam numpy ndarray of shape (M,N) of N warping functions with M samples
- alpha quantile value (e.g.,=.05, i.e., 95%)
- **k\_a** scalar for outlier cutoff (e.g.,=1)

**Return type** tuple of numpy array

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

functions with M samples :return Q1: First quartile :return Q3: Second quartile :return Q1a: First quantile based on alpha :return Q3a: Second quantile based on alpha :return minn: minimum extreme function :return maxx: maximum extreme function :return outlier\_index: indexes of outlier functions :return median\_x: median warping function :return psi median: median srsf of warping function :return plt: surface plot mesh

## **GAUSSIAN GENERATIVE MODELS**

Gaussian Model of functional data

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

```
gauss_model.gauss_model (fn, time, qn, gam, n=1, sort_samples=False)
```

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

## **Parameters**

- **fn** (np.ndarray) numpy ndarray of shape (M,N) of N aligned functions with M samples
- time (np.ndarray) vector of size M describing the sample points
- qn (np.ndarray) numpy ndarray of shape (M,N) of N aligned srvfs with M samples
- gam (np.ndarray) warping functions
- n (integer) number of random samples
- sort samples (bool) sort samples (default = T)

**Return type** tuple of numpy array

Return fs random aligned samples

Return gams random warping functions

**Return ft** random samples

```
gauss_model.joint_gauss_model(fn, time, qn, gam, q0, n=1, no=3)
```

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

## **Parameters**

- **fn** (np.ndarray) numpy ndarray of shape (M,N) of N aligned functions with M samples
- time (np.ndarray) vector of size M describing the sample points
- qn (np.ndarray) numpy ndarray of shape (M,N) of N aligned srsfs with M samples
- gam (np.ndarray) warping functions
- q0 numpy ndarray of shape (M,N) of N unaligned srsfs with samples
- n (integer) number of random samples
- **n** number of principal components (default = 3)

Return type tuple of numpy array

**Return fs** random aligned samples

**Return gams** random warping functions

**Return ft** random samples

**CHAPTER** 

**FIVE** 

## **FUNCTIONAL PRINCIPAL LEAST SQUARES**

Partial Least Squares using SVD

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

fPLS.pls\_svd(time, qf, qg, no, alpha=0.0)

This function computes the partial least squares using SVD

## **Parameters**

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

Return type numpy ndarray

Return wqf f weight function

Return wqg g weight function

Return alpha smoothing value

Return values singular values

## **ELASTIC REGRESSION**

Warping Invariant Regression using SRSF

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

regression.elastic\_logistic (f, y, time, B=None, df=20,  $max\_itr$ =20, cores=-1, smooth=False)

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

## **Parameters**

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

**Return type** tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

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

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

```
regression.elastic_mlogistic (f, y, time, B=None, df=20, max\_itr=20, cores=-1, delta=0.01, par-allel=True, smooth=False)
```

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

## **Parameters**

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

• cores – number of cores for parallel processing (default all)

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

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

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

regression.elastic\_prediction(f, time, model, y=None, smooth=False)

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

#### **Parameters**

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

Return type tuple of numpy array

Return alpha alpha parameter of model

Return beta beta(t) of model

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

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

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

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

## **Parameters**

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

**Return type** tuple of numpy array

**Return alpha** alpha parameter of model

Return beta beta(t) of model

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

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

regression.logistic\_warp (beta, time, q, y) calculates optimal warping for function logistic regression

#### **Parameters**

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

Return type numpy array

Return gamma warping function

regression.logit\_gradient (b, X, y) calculates gradient of the logistic loss

#### **Parameters**

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

Return type numpy array

Return grad gradient of logisitc loss

regression.logit\_hessian (s, b, X, y) calculates hessian of the logistic loss

#### **Parameters**

- $\mathbf{s}$  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
- $\mathbf{q}$  numpy ndarray of shape (M,N) of N functions with M samples
- y numpy ndarray of shape (1,N) responses
- max\_itr maximum number of iterations (Default=8000)
- tol stopping tolerance (Default=1e-10)
- **delta** gradient step size (Default=0.008)
- **display** display iterations (Default=0)

**Return type** tuple of numpy array

Return gam\_old warping function

```
regression.phi(t)
```

calculates logistic function, returns  $1/(1 + \exp(-t))$ 

**Parameters** t – scalar

Return type numpy array

Return out return value

regression.regression\_warp (*beta*, *time*, *q*, *y*, *alpha*) calculates optimal warping for function linear regression

## **Parameters**

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

responses :param alpha: numpy scalar

Return type numpy array

Return gamma\_new warping function

## **ELASTIC PRINCIPAL COMPONENT REGRESSION**

Warping PCR Invariant Regression using SRSF

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

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

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

## **Parameters**

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

**Return type** tuple of numpy array

Return alpha alpha parameter of model

Return b regressor vector

**Return y** response vector

**Return warp\_data** alignment object from srsf\_align

**Return pca** fpca object from corresponding pca method

Return Loss logistic loss

Return pca.method string of pca method

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

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

#### **Parameters**

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

- pca\_method string specifing pca method (options = "combined", "vert", or "horiz", default = "combined")
- **no** scalar specify number of principal components (default=5)
- **smooth\_data** smooth data using box filter (default = F)
- **sparam** number of times to apply box filter (default = 25)

**Return type** tuple of numpy array

Return alpha alpha parameter of model

Return b regressor vector

**Return y** response vector

Return warp\_data alignment object from srsf\_align

Return pca fpca object from corresponding pca method

Return Loss logistic loss

Return pca.method string of pca method

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

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

## **Parameters**

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

**Return type** tuple of numpy array

Return alpha alpha parameter of model

**Return b** regressor vector

Return y response vector

**Return warp\_data** alignment object from srsf\_align

Return pca fpca object from corresponding pca method

**Return SSE** sum of squared errors

Return pca.method string of pca method

## **ELASTIC FUNCTIONAL TOLERANCE BOUNDS**

Functional Tolerance Bounds using SRSF

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

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

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

## **Parameters**

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

Return type tuple of boxplot objects

Return amp amplitude tolerance bounds

Return ph phase tolerance bounds

tolerance.mvtol\_region (x, alpha, P, B)

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

## **Parameters**

- $\mathbf{x} (M,N)$  matrix defining N variables of M samples
- alpha confidence level
- **P** coverage level
- **B** number of bootstrap samples

Return type double

Return tol tolerance factor

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

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

## **Parameters**

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

Return type tuple of boxplot objects

Return warp alignment data from time\_warping

Return pca functional pca from jointFPCA

Return tol tolerance factor

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

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

If positive, int\_like or int-convertible 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 (if any of the  $d_i$  are floats, they are first converted to integers by truncation). A single float randomly sampled from the distribution is returned if no argument is provided.

This is a convenience function. If you want an interface that takes a tuple as the first argument, use numpy.random.standard normal instead.

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

standard\_normal: Similar, but takes a tuple as its argument.

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

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

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

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

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

tolerance.rwishart (df, p)

## **Parameters**

- df degree of freedom
- p number of dimensions

Return type double

Return R matrix

## SRVF GEODESIC COMPUTATION

geodesic calculation for SRVF (curves) open and closed)

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

 ${\tt geodesic.back\_parallel\_transport}~(u1, alpha, basis, T=100, k=5)$ 

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

Return type numpy ndarray

Return utilde translated vector

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

**Return type** numpy ndarray

Return alphadot derivative of alpha

geodesic.calculate\_energy (alphadot, T=100, k=5) calculates energy along path

## **Parameters**

- alphadot numpy ndarray of shape (2,M) of M samples
- $\mathbf{T}$  Number of samples of curve (Default = 100)
- $\mathbf{k}$  number of samples along path (Default = 5)

**Return type** numpy scalar

## **Return E** energy

geodesic.calculate\_gradE (u, utilde, T=100, k=5) calculates gradient of energy along path

#### **Parameters**

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

Return type numpy scalar

Return gradE gradient of energy

Return normgradE norm of gradient of energy

geodesic.cov\_integral (alpha, alphadot, basis, T=100, k=5)

Calculates covariance along path alpha

#### **Parameters**

- alpha numpy ndarray of shape (2,M) of M samples (first curve)
- alphadot numpy ndarray of shape (2,M) of M samples
- basis list numpy ndarray of shape (2,M) of M samples
- $\mathbf{T}$  Number of samples of curve (Default = 100)
- $\mathbf{k}$  number of samples along path (Default = 5)

Return type numpy ndarray

Return u covariance

## geodesic.find\_basis\_normal\_path(alpha, k=5)

computes orthonormalized basis vectors to the normal space at each of the k points (q-functions) of the path alpha

## **Parameters**

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

Return type numpy ndarray

**Return basis** basis vectors along the path

```
geodesic.geod_dist_path_strt(beta, k=5)
```

calculate geodisc distance for path straightening

## **Parameters**

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

Return type numpy scalar

Return dist geodesic distance

```
geodesic.geod sphere(beta1, beta2, k=5)
```

This function caluclates the geodecis between open curves beta1 and beta2 with k steps along path

## **Parameters**

- beta1 numpy ndarray of shape (2,M) of M samples
- beta2 numpy ndarray of shape (2,M) of M samples
- $\mathbf{k}$  number of samples along path (Default = 5)

Return type numpy ndarray

Return dist geodesic distance

Return path geodesic path

Return O rotation matrix

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

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

## **Parameters**

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

Return type numpy ndarray

**Return alpha** a path between two q-functions

Return beta a path between two curves

Return O rotation matrix

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

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

## **Parameters**

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

**Return type** numpy ndarray

Return alpha a path between two q-functions

Return beta a path between two curves

Return O rotation matrix

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

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

## **Parameters**

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

- **beta2** numpy ndarray of shape (2,M) of M samples (end curve)
- **betamid** numpy ndarray of shape (2,M) of M samples (mid curve Default = NULL, only needed for init "rand")
- init initilizae path geodesic or random (Default = "rand")
- **T** Number of samples of curve (Default = 100)
- $\mathbf{k}$  number of samples along path (Default = 5)

**Return type** numpy ndarray

Return dist geodesic distance

Return path geodesic path

Return pathsque geodesic path sequence

Return E energy

 $\verb|geodesic.update_path| (alpha, beta, gradE, delta, T=100, k=5)$ 

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

Return type numpy scalar

Return alpha updated path of srvfs

Return beta updated path of curves

## **CHAPTER**

## TEN

## **UTILITY FUNCTIONS**

Utility functions for SRSF Manipulations

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

utility\_functions.SqrtMean(gam)

calculates the srsf of warping functions with corresponding shooting vectors

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

Return type 2 numpy ndarray and vector

Return mu Karcher mean psi function

**Return gam\_mu** vector of dim N which is the Karcher mean warping function

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

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

utility\_functions.SqrtMeanInverse(gam)

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

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

Return type vector

Return gamI inverse of gam

utility functions. SqrtMedian (gam)

calculates the median srsf of warping functions with corresponding shooting vectors

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

Return type 2 numpy ndarray and vector

Return gam\_median Karcher median warping function

Return psi\_meidan vector of dim N which is the Karcher median srsf function

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

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

utility\_functions.cumtrapzmid(x, y, c, mid)

cumulative trapezoidal numerical integration taken from midpoint

## **Parameters**

- $\mathbf{x}$  vector of size N describing the time samples
- y vector of size N describing the function
- c midpoint

• mid – midpiont location

Return type vector

Return fa cumulative integration

utility\_functions.diffop(n, binsize=1)

Creates a second order differential operator

#### **Parameters**

- n dimension
- binsize dx (default = 1)

Return type numpy ndarray

**Return m** matrix describing differential operator

utility\_functions.elastic\_distance(f1, f2, time, lam=0.0)

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

#### **Parameters**

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

Return type scalar

Return Dy amplitude distance

Return Dx phase distance

utility\_functions.f\_K\_fold(Nobs, K=5)

generates sample indices for K-fold cross validation

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

**Return type** numpy ndarray

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

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

utility\_functions.**f\_to\_srsf** (*f*, *time*, *smooth=False*) converts f to a square-root slope function (SRSF)

## **Parameters**

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

Return type vector

**Return q** srsf of f

utility\_functions.geigen(Amat, Bmat, Cmat)
generalized eigenvalue problem of the form

max 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
- £ 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='DP', lam=0.0, f1o=0.0, f2o=0.0) calculates the warping to align srsf q2 to q1

#### **Parameters**

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

Return type vector

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

utility\_functions.optimum\_reparam\_pair (q, time, q1, q2, lam=0.0) calculates the warping to align srsf pair q1 and q2 to q

#### **Parameters**

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

## Return type vector

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

utility\_functions.outlier\_detection (q, time, mq, k=1.5) calculates outlier's using geodesic distances of the SRSFs from the median

## **Parameters**

- **q** numpy ndarray of N x M of M SRS functions with N samples
- time vector of size N describing the sample points
- mq median calculated using time\_warping.srsf\_align()
- $\mathbf{k}$  cutoff threshold (default = 1.5)

**Returns** q\_outlier: outlier functions

utility\_functions.randomGamma (gam, num)
generates random warping functions

## **Parameters**

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

Returns rgam: random warping functions

utility\_functions.resamplefunction (x, n) resample function using n points

#### **Parameters**

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

**Return type** numpy array

Return xn resampled function

utility\_functions.rgam(N, sigma, num)
Generates random warping functions

## **Parameters**

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

**Returns** gam: numpy ndarray of warping functions

```
utility_functions.smooth_data(f, sparam)
```

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.update_progress(progress)
```

This function creates a progress bar

Parameters progress – fraction of progress

```
utility_functions.warp_f_gamma (time, f, gam) warps a function f by gam
```

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

Return type numpy ndarray

Return f\_temp warped srsf

```
utility_functions.warp_q_gamma(time, q, gam) warps a srsf q by gam
```

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

Return type numpy ndarray

Return q temp warped srsf

```
utility_functions.zero_crossing (Y, q, bt, time, y\_max, y\_min, gmax, gmin) finds zero-crossing of optimal gamma, gam = s*gmax + (1-s)*gmin from elastic regression model
```

#### **Parameters**

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

- gmax max warping function
- gmin min warping fucntion

Return type numpy array

Return gamma optimal warping function

### **CHAPTER**

## **ELEVEN**

## **CURVE FUNCTIONS**

functions for SRVF curve manipulations

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

curve\_functions.calc\_j(basis)

Calculates Jacobian matrix from normal basis

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

Return type numpy ndarray

Return j Jacobian

curve\_functions.calculate\_variance(beta)

This function calculates variance of curve beta

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

Return type numpy ndarray

Return variance variance

curve functions.calculatecentroid(beta)

This function calculates centroid of a parameterized curve

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

**Return type** numpy ndarray

Return centroid center coordinates

 $\verb|curve_functions.curve_to_q| (\textit{beta})$ 

This function converts curve beta to srvf q

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

Return type numpy ndarray

**Return q** srvf of curve

curve\_functions.curve\_zero\_crossing(Y, beta, bt, y\_max, y\_min, gmax, gmin)

finds zero-crossing of optimal gamma, 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.find\_basis\_normal(q)

Finds the basis normal to the srvf

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

**Return type** list of numpy ndarray

Return basis list containing basis vectors

## curve\_functions.find\_best\_rotation (q1, q2)

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

### **Parameters**

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

Return type numpy ndarray

Return q2new optimal rotated q2 to q1

Return R rotation matrix

## curve\_functions.find\_rotation\_and\_seed\_coord(beta1, beta2)

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

#### **Parameters**

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

Return type numpy ndarray

Return beta2new optimal rotated beta2 to beta1

Return O rotation matrix

Return tau seed

### curve\_functions.find\_rotation\_and\_seed\_q(q1, q2)

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

#### **Parameters**

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

**Return type** numpy ndarray

Return beta2new optimal rotated beta2 to beta1

Return O rotation matrix

Return tau seed

```
curve functions.gram schmidt (basis)
```

Performs Gram Schmidt 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**

- $\mathbf{f}$  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)
```

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

#### **Parameters**

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

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

**Return type** numpy ndarray

Return v shooting vectors

Return dist distance

curve\_functions.optimum\_reparam\_curve (q1, q2, lam=0.0) calculates the warping to align srsf q2 to q1

#### **Parameters**

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

Return type vector

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

curve\_functions.parallel\_translate(w, q1, q2, basis, mode=0) parallel translates q1 and q2 along manifold

#### **Parameters**

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

Return type numpy ndarray

Return wbar translated vector

curve\_functions.pre\_proc\_curve(beta, T=100)

This function prepcoessed a curve beta to set of closed curves

#### **Parameters**

- beta numpy ndarray of shape (2,M) of M samples
- $\mathbf{T}$  number of samples (default = 100)

Return type numpy ndarray

Return betanew projected beta

Return quew 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
- $\mathbf{q}$  numpy ndarray of shape (2,M) of M samples
- basis list of numpy ndarray of shape (2,M) of M samples

Return type numpy ndarray

Return wproj projected q

curve\_functions.psi (x, a, q)

This function formats variance output

#### **Parameters**

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

Return type numpy ndarray

Return psi1 variance

Return psi2 cross variance

Return psi3 curve end

Return psi4 curve end

curve\_functions.q\_to\_curve(q)

This function converts srvf to beta

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

Return type numpy ndarray

Return beta parameterized curve

curve\_functions.resamplecurve(x, N=100)

This function resamples a curve to have N samples

#### **Parameters**

- $\mathbf{x}$  numpy ndarray of shape (2,M) of M samples
- N Number of samples for new curve (default = 100)

Return type numpy ndarray

Return xn resampled curve

curve\_functions.scale\_curve(beta)

scales curve to length 1

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

Return type numpy ndarray

Return beta\_scaled scaled curve

Return scale scale factor used

curve\_functions.**shift\_f** (*f*, *tau*) shifts a curve f by tau

#### **Parameters**

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

Return type numpy ndarray

Return fn shifted curve

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