# pyEDM Version 2.2.3 August 7, 2025

<u>pyEDM</u> is a Python package of empirical dynamic modeling (EDM) algorithms. Input data are Pandas DataFrame, return objects are Pandas DataFrame, Python dictionaries of Pandas DataFrame, or the class object of the algorithm. pyEDM is hosted on the Python Package Index (PyPI) at <u>pypi/pyEDM</u>. A Jupyter notebook GUI is available at <u>ipyEDM</u>.

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# Introduction

pyEDM is a Python package implementing empirical dynamic modeling (EDM) algorithms. Input and output objects are based on Pandas DataFrame. Core algorithms are listed in Table 1.

Version 2. is a pure Python implementation based on numpy replacing the C++ kernel in Version 1.

Algorithm	API Interface	Reference
Simplex projection	Simplex()	Sugihara and May (1990)
Sequential Locally Weighted Global Linear Maps (S-map)	SMap()	<u>Sugihara (1994)</u>
Predictions from multivariate embeddings	<pre>Simplex(), SMap()</pre>	<u>Dixon et. al. (1999)</u>
Convergent cross mapping	CCM()	Sugihara et. al. (2012)
Multiview embedding	Multiview()	Ye and Sugihara (2016)

Convenience functions to prepare and evaluate data are listed in Table 2. The functions EMbedDimension(), PredictInterval(), PredictNonlinear() use multiprocessing for parallelism.

Function	Purpose Default Parameters	
Embed()	Timeseries delay dimensional embedding	
EmbedDimension()	Evaluate prediction skill vs. embedding dimension	E = [1, 10]
PredictInterval()	Evaluate prediction skill vs. forecast interval	Tp = [1, 10]
PredictNonlinear()	Evaluate prediction skill vs. SMap nonlinear localization	θ = 0.01, 0.1, 0.3, 0.5, 0.75, 1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9
ComputeError()	Pearson ρ, RMSE, MAE, CAE	
SurrogateData()	Generate random surrogates	
Examples()	Example function calls and plots	

API wrapper applications/functions for common tasks can be found in the apps/ directory as listed in Table 3. The Python file can be run as a command line application with command line options, or, loaded as a module and the function called directly allowing access to all return values.

Application / Function	Purpose
CCM_Matrix.py	CCM matrix of all columns vs. all columns. Compute linear slope and optional nonlinear convergence functions.
CrossMap_Columns.py	Simplex cross map all columns against target.
CrossMap_ColumnList.py	Simplex cross map list of columns against a target. Columns can be a list of single columns, or list of multiple columns.
CrossMap_Matrix.py	Simplex cross map all columns vs. all columns.
EmbedDim_Columns.py	Process parallelize EmbedDimension() to find maximum rho, E for all columns.
Embedding.py	Extend Embed() to create mixed multivariate embeddings allowing positive and negative lags. Useful to create mixed multivariate embeddings for SMap().
SMap_theta.py	Process parallelize SMap() over a list of theta.
SMap_Tp.py	Process parallelize SMap() over a list of Tp.

## Installation

## Python Package Index (PyPI)

```
pyEDM is available at <a href="mailto:pyEDM/">pyEDM / ...</a>
```

```
Installation: python -m pip install pyEDM
```

### Local Install

pyEDM can be installed from the github archive.

- 1) Download pyEDM: git clone <a href="https://github.com/SugiharaLab/pyEDM">https://github.com/SugiharaLab/pyEDM</a>
- 2) Build and install package in pyEDM directory: python -m pip install .

## Example Usage

```
>>> import pyEDM
>>> pyEDM.Examples()
```

See the Examples section below.

## Data Requirements

Input data files are required to be a Pandas DataFrame.

DataFrames are required to have column names.

**It is expected the first column is a vector of times or time indices.** This can be disabled with the noTime = True parameter.

The data are expected to be sequential time series observations. NaN data will be removed if ignoreNan = True, the default. If NaN are present they will propagate through the nearest neighbors resulting in NaN for any result involving a NaN neighbor.

Parameters
API parameter names and purpose are listed in Table 3.

Parameter	Type	Default	Purpose
dataFrame	Pandas DataFrame	None	Input DataFrame
columns	[] or string	" "	Column names or indices for library
target	[] or string	" "	Target library column name or index
lib	[] or string	" "	library start : stop row indices
pred	[] or string	" "	prediction start : stop row indices
D	int	0	Multiview state-space dimension
E	int	0	Embedding dimension
Тр	int	0 or 1	Prediction interval
knn	int	0	Number nearest neighbors
tau	int	-1	Embedding delay
theta	float	0	SMap localization
exclusionRadius	int	0	Prediction vector exclusion radius
embedded	bool	False	Is data an embedding?
ignoreNan	bool	True	Remove nan from lib & target
validLib	[ bool ]	[]	Conditional Embedding (CE)
noTime	bool	False	Do not require first column to be time
generateSteps	int	0	Generative mode (Simplex, SMap)
generateConcat	bool	False	Merge original and generated data
solver	sklearn.linear_model	None	SMap solver
libSizes	[ int ] or string	[]	CCM library sizes
sample	int	0	CCM number of random samples
includeData	bool	False	CCM include all statistics in return
seed	unsigned	0	CCM RNG seed, $0 = \text{random seed}$
multiview	int	0	Number of ensembles, $0 = \text{sqrt}(N)$
trainLib	bool	True	Multiview use lib as training library
excludeTarget	bool	True	Multiview exclude target from combos
method	string	"ebisusaki'	' SurrogateData method
alpha	float	range / 5	SurrogateData seasonal noise std dev
smooth	float	0.8	SurrogateData seasonal spline smooth
verbose	bool	False	Echo messages

# Application Programming Interface (API)

## Embed

Create a time-delay embedding from each of the columns in the dataFrame or csv dataFile.

```
Embed ( dataFrame = None,

E = 0,

tau = -1,

columns = "",

includeTime = False,

pathIn = "./",

dataFile = "" )
```

Return: DataFrame with time shifted values dictated by E and tau.

Note: The returned DataFrame will not have the time column unless includeTime = True.

## Simplex

Simplex projection of the input DataFrame columns to the target.

```
Simplex ( dataFrame
                           = None,
          columns
                           = ""
          target
                           = ""
          lib
                           = ""
          pred
          Е
                           = 0,
          Тр
                           = 1,
          knn
                           = 0,
          tau
                           = -1,
          exclusionRadius = 0,
                           = False,
          embedded
                           = [],
          validLib
          noTime
                           = False,
          generateSteps
                           = 0,
          generateConcat = False,
          verbose
                           = False,
          showPlot
                           = False,
          ignoreNan
                           = True,
          returnObject
                           = False )
```

### Return:

If returnObject = False: returns DataFrame with columns: "Time", "Observations", "Predictions", "Pred\_Variance".

If returnObject = True: the Simplex class object is returned. The attribute Projection contains the simplex projection DataFrame.

### **Parameters**

lib and pred specify [start stop] row indices of the input data for the library and predictions.

If embedded is False all data columns are embedded to dimension E with delay tau. If embedded is True the data columns are assumed to be an embedding.

If knn is not specified, and embedded is False, it is set equal to E+1. If embedded is True, knn is set equal to the number of columns + 1.

exclusionRadius defines the number of library rows excluded from the state-space library with respect to a temporal "radius" from the prediction state. If exclusionRadius = 1, library state-space points from observation time series that are within  $\pm 1$  sequential observation row of the prediction state are not included in the library. Note that units of the radius are time series rows, not time values.

validLib implements conditional embedding (CE). It is a boolean vector the same length as the number of time series rows. A False entry means that the state-space vector derived from the corresponding time series row will not be included in the state-space library.

If noTime = False, the first column of the input DataFrame or .csv file must be an index or time column. If noTime = True an index time column is created.

If generateSteps > 0 data are generated from the specified library. The prediction indices (pred) are overridden to generate one prediction at the end of the library. Generative mode only works on univariate (columns == target) data with embedded = False.

If generateConcat is True data are generated from the specified library are appended to the input dataFrame Observations.

## **SMap**

SMap projection of the input data file or DataFrame. See the Parameters table for parameter definitions.

```
SMap( dataFrame
                     = None,
                    = ""
     columns
                    = ""
     target
                    = ""
     lib
                    = ""
     pred
                     = 0,
     Ε
                    = 1,
     Tp
                    = 0,
     knn
     tau
                    = -1,
     theta
                    = 0,
     exclusionRadius = 0,
                    = None,
     solver
     embeddeu
validLib = [],
= Fal
                   = False,
     embedded
                   = False,
     generateSteps = 0,
     generateConcat = False,
     ignoreNan = True,
     showPlot
                   = False,
     verbose
                    = False,
     returnObject
                    = False )
```

### Return:

dict with three DataFrames:

The predictions DataFrame has 3 columns "Time", "Observations", "Predictions", "Pred\_Variance". nan values are inserted where there is no observation or prediction.

The coefficients DataFrame will have E+2 columns. The first column is the "Time" vector, the remaining E+1 columns are the SMap SVD fit coefficients. The first column "C0" is the bias term, following coefficients are  $\partial$  target /  $\partial$  columns[i].

The singularValues DataFrame holds SVD singular values if the default LAPACK solver, or scikit.learn solver is used. The scikit.learn LinearRegression does not return a singular value for the intercept (bias) term.

If returnObject = True, the SMap class object is returned. The attribute Projection contains the simplex projection DataFrame, Coefficients and SingularValues the corresponding DataFrames.

### **Parameters**

lib and pred specify [start, stop] row indices of the input data for the library and predictions.

If embedded is False the data columns are embedded to dimension E with delay tau. If embedded is True the data columns are assumed to be a multivariable data block.

If columns is a string and column names have whitespace place the column names in a list.

If a multivariate data set is used (number of columns > 1) it must use embedded = true with E equal to the number of columns. This prevents the function from internally time-delay embedding the multiple columns to dimension E. If the internal time-delay embedding is performed, then state-space columns will not correspond to the intended dimensions in the matrix inversion, coefficient assignment, and prediction. In the multivariate case, the user should first prepare the embedding (using Embed() for time-delay embedding if desired), then pass this embedding to SMap with appropriately specified columns, E, and embedded = true.

If knn is not specified, it is set equal to the library size. If knn is specified, it must be greater than E+1.

exclusionRadius defines the number of library rows excluded from the state-space library with respect to a temporal "radius" from the prediction state. If exclusionRadius = 1, library state-space points from observation time series that are within  $\pm 1$  sequential observation row of the prediction state are not included in the library. Note that units of the radius are time series rows, not time values.

If noTime = False, the first column of the input DataFrame or .csv file must be an index or time column. If noTime = True an index or time column is not required.

ignoreNan removes nan to avoid nan observations and associated state vectors. If ignoreNan is False no nan are removed. The user can manually specify library row segments to ignore nan values.

validLib implements conditional embedding (CE). It is a boolean vector the same length as the number of time series rows. A False entry means that the state-space vector derived from the corresponding time series row will not be included in the state-space library.

The default solver for the SMap coefficient matrix is SciPy scipy.linalg.lstsq. This is a wrapper for the LAPACK function dgelsd().

The solver can be replaced with a user-instantiated class object from the python sklearn.linear\_model: Linear Models. Supported solvers include: LinearRegression, SGDRegressor, Ridge, Lasso, LassoLars, OrthogonalMatchingPursuit, ElasticNet, RidgeCV, LassoCV, ElasticNetCV... See the pyEDM/tests/smapSolverTest.py script for examples.

If generateSteps > 0 data are generated from the specified library. The prediction indices (pred) are overridden to generate one prediction at the end of the library. Generative mode only works on univariate (columns == target) data with embedded = False. If generateConcat is True data are generated from the specified library are appended to the input dataFrame Observations.

### **CCM**

Convergent cross mapping of columns against target via Simplex. Normally, one column and one target are specified. The column time series is time-delay embedded to dimension E, cross mapped with the target time series. The target time series is then embedded to E and cross mapped against the column as the "target" time series.

```
CCM( dataFrame
                        = None,
     columns
                        = ""
     target
     libSizes
     sample
                        = 0,
     Ε
                        = 0,
                        = 0,
     Тр
                        = 0,
     knn
     tau
                        = -1,
     exclusionRadius = 0.
     seed
                        = None,
     seeu
embedded
validLib
includeData
                       = False,
                        = [],
                        = False,
     noTime
                        = False,
     ignoreNan
verbose
showPlot
returnObject
                        = True,
                        = False,
                        = False,
                        = False )
```

#### Return:

DataFrame with LibSize, column:target and target:column CCM correlations.

If includeData is True, a dict is returned with the LibMeans DataFrame, and a DataFrame with prediction statistics of all predictions in each ensemble.

If there are multiple columns and embedded is false, each column is time-delay embedded to dimension E creating an N-columns \* E dimensional "mixed" embedding. If embedded is true, no time-delay embedding is done, creating a multivariate embedding of the speficied columns. The same logic applies if multiple target are specified for the "reverse" mapping. If embedded is false, each target is time-delay embedded to dimension E creating an N-target \* E dimensional "mixed" embedding cross mapped to the first column as the cross map target. If embedded is true, no time-delay embedding is done, creating a multivariate embedding of the speficied target(s).

Cross mappings are performed between column : target, and, target : column in separate multiprocessing instances. If additional multiprocessing is applied, halve the number of processors.

The CCM\_Matrix.py application in apps/uses ProcessPoolExecutor to process parallelize CCM. All dataFrame columns are cross mapped to all others. A convergence metric is computed based on linear slope of the CCM( libSize ).

### **Parameters**

The libSizes parameter is list of library sizes or a string of whitespace or comma separated library sizes. If the list has 3 values, and, if the third value is less than the second value, the three values are interpreted as a sequence generator specifying "start stop increment" row values, i.e. "10 80 10" will evaluate library sizes from 10 to 80 in increments of 10.

If noTime = False, the first column of the input DataFrame or .csv file must be an index or time column. If noTime = True an index or time column is not required.

Note: The entire prediction vector is used in the Simplex prediction at each library subset size.

### Multiview

Multiview embedding and forecasting of DataFrame columns.

```
Multiview( dataFrame
                                = None,
             columns
                                = ""
             target
                                = ""
             lib
                                = ""
             pred
                                = 0,
             D
             Е
                                = 1,
                                = 1,
             Тр
             knn
                                = 0,
             tau
                                = -1,
             multiview
                               = 0,
             exclusionRadius = 0,
             trainLib = True,
             excludeTarget = False,
            noTime = False
ignoreNan = True,
verbose = False
numProcess = 4,
showPlot = False
                              = False,
                               = False,
                                = False,
             returnObject
                               = False )
```

### Return:

The Predictions DataFrame has 4 columns "Time", "Observations", "Predictions", "Pred Variance".

The View DataFrame will have 4 columns. The first column are tuples of column names for each multiview. The following three columns are "rho", "MAE", "RMSE" corresponding to the prediction Pearson correlation, maximum absolute error and root mean square error.

### **Parameters**

D represents the number of variables to combine for each assessment, if not specified, it is the number of columns.

E is the embedding dimension of each variable. If E = 1, no time delay embedding is done.

multiview is the number of top-ranked D-dimensional predictions to average for the final prediction. Corresponds to parameter k in Ye & Sugihara with default  $k = \operatorname{sqrt}(C)$  where C is the number of combinations C(n,D) available from the embedding columns taken D at-a-time.

trainLib specifies whether projections used to rank the column combinations are done in-sample (pred = lib, the default), or, using the lib and pred specified as input options (trainLib False).

lib and pred specify [start, stop] row indices of the input data for the library and predictions.

If knn is not specified, it is set equal to D+1.

numProcess defines the number of multiprocessing instances.

If noTime = False, the first column of the input DataFrame or .csv file must be an index or time column. If noTime = True an index or time column is not required.

## EmbedDimension

Evaluate Simplex prediction skill for embedding dimensions from 1 to maxE.

```
EmbedDimension( dataFrame
                              = None,
                              = "".
               columns
                              = "",
               target
                              = 10,
               maxE
                              = ""
               lib
                              = ""'
               pred
               Тр
               tau
                              = -1,
               exclusionRadius = 0,
               embedded
                              = False,
                              = [],
               validLib
               noTime
                              = False,
               ignoreNan
                              = True,
                              = False,
               verbose
               numProcess
                              = 4,
                              = True )
               showPlot
```

Return: DataFrame with columns "E" and "rho".

Note: Python multiprocessing is used to process parallelize over the embedding dimensions from 1 to maxE. numProcess defines the number of multiprocessing instances.

## PredictInterval

Evaluate Simplex prediction skill for forecast intervals from 1 to maxTp.

```
PredictInterval( dataFrame
                                 = None,
                                = "",
                 columns
                                = ""
                 target
                 lib
                                = "".
                 pred
                 maxTp
                                = 10,
                 Ε
                                 = -1,
                 exclusionRadius = 0,
                 embedded
                                = False,
                 validLib
                                = [],
                 noTime
                                = False,
                 ignoreNan
                                = True,
                 verbose
                                = False,
                 numProcess
                                = 4,
                 showPlot
                                = True)
```

Return: DataFrame with columns "Tp" and "rho".

Note: Python multiprocessing is used to process parallelize over the forecast intervals from 1 to maxTp. numProcess defines the number of multiprocessing instances.

### PredictNonlinear

Evaluate SMap prediction skill for localization parameter  $\theta$ .

```
PredictNonlinear( dataFrame
                                 = None,
                                = "",
                 columns
                 target
                 theta
                                 = None,
                 lib
                                  "",
                 pred
                                 = 1,
                 Е
                                 = 1,
                 Тр
                                 = 0,
                 knn
                 tau
                 exclusionRadius = 0,
                 solver
                                 = None,
                 embedded
                                 = False,
                 validLib
                                = [],
                 noTime
                                = False,
                 ignoreNan
                                = True,
                                 = False,
                 verbose
                                = 4,
                 numProcess
                                 = True )
                 showPlot
```

Return: DataFrame with columns "theta" and "rho".

If knn is not specified, it is set equal to the library size. If knn is specified, it must be greater than E.

Note: Python multiprocessing is used to process parallelize over the localization parameter theta. numProcess defines the number of multiprocessing instances.

# Compute Error

Compute Pearson correlation coefficient, maximum absolute error (MAE), cumulative absolute error (CAE) and root mean square error (RMSE) between two vectors. A minimum of 5 data points is required. Any nan will be removed.

```
ComputeError( obsIn, predIn, digits = 6 )
```

Return:

```
dict { rho : double,
     MAE : double,
     CAE : double,
     RMSE : double, }
```

## SurrogateData

Generate surrogate data using one of three methods.

```
SurrogateData( dataFrame = None, column = None, method = 'ebisuzaki', numSurrogates = 10, alpha = None, smooth = 0.8, outputFile = None )
```

### Return:

DataFrame with numSurrogates + 1 columns. First column is time vector from the input dataFrame. Remaining numSurrogates columns are the surrogate data with column names appended with \_1, \_2... for each surrogate.

### **Parameters**

#### method:

1) random\_shuffle

Sample the data with a uniform distribution.

### 2) ebisuzaki

A Method to Estimate the Statistical Significance of a Correlation When the Data Are Serially Correlated. Journal of Climate.

https://doi.org/10.1175/1520-0442(1997)010<2147:AMTETS>2.0.CO;2

Presumes data are serially correlated with low pass coherence. The method implements "resampling in the frequency domain. This procedure will not preserve the distribution of values but rather the power spectrum (periodogram). The advantage of preserving the power spectrum is that resampled series retains the same autocorrelation as the original series."

### 3) seasonal

Presume a smoothing spline represents the seasonal trend. The smooth parameter can range from 0 to 1. See <u>scipy.interpolate.UnivariateSpline</u> parameter s.

Each surrogate is a summation of the trend, resampled residuals, and possibly additive Gaussian noise. Default noise has a standard deviation (alpha) that is the data range / 5.

Note: It is presumed the first column of the dataFrame is a time vector. It is set as the first column of the returned DataFrame.

# **Application Notes**

Input data files are Pandas DataFrame.

The DataFrame are required to have column names.

**It is expected the first column is a vector of times or time indices.** This can be disabled by setting the parameter noTime = True.

If columns is a string and column names have whitespace place the column names in a list.

SMap () should be called with DataFrame that have columns explicitly corresponding to dimensions E. This means that if a multivariate data set is used, it should Not be called with an embedding from Embed() since Embed() will add lagged coordinates for each variable. These extra columns will not correspond to the intended dimensions in the matrix inversion and prediction reconstruction rendering the SMap coefficients invalid. In this case, use the embedded parameter set to True in SMap() so columns correspond to the proper dimension.

## **Examples**

```
from pyEDM import *
df = EmbedDimension( dataFrame = sampleData["TentMap"],
                    columns = "TentMap", target = "TentMap",
                    lib = [1, 100], pred = [201, 500],
                    showPlot = True )
df = PredictInterval( dataFrame = sampleData["TentMap"],
                     columns = "TentMap", target = "TentMap",
                     lib = [1, 100], pred = [201, 500],
                     E = 2, showPlot = True )
df = PredictNonlinear( dataFrame = sampleData["TentMapNoise"],
                      columns = "TentMap", target = "TentMap",
                      lib = [1, 100], pred = [201, 500],
                      E = 2, showPlot = True )
df = Simplex( dataFrame = sampleData["block_3sp"],
             columns = "x_t y_t z_t", target = "x_t",
             lib = [1, 99], pred = [100, 198], E = 3,
             embedded = True, showPlot = True )
df = Simplex( dataFrame = sampleData["block_3sp"],
             columns = "x_t", target = "x_t",
             lib = [1, 99], pred = [100, 195], E = 3,
             showPlot = True )
lib = [1, 100], pred = [101, 198], E = 3,
               trainLib = False, showPlot = True )
S = SMap( dataFrame = sampleData["circle"],
          columns = ["x", "y"], target = "x",
          lib = [1, 100], pred = [101, 198],
          E = 2, theta = 4, embedded = True,
          showPlot = True )
df = CCM( dataFrame = sampleData["sardine_anchovy_sst"],
          E = 3, Tp = 0, columns = "anchovy", target = "np_sst",
          libSizes = [10, 70, 10], sample = 100, showPlot = True )
```

## References

Dixon, P. A., M. Milicich, and G. Sugihara, 1999. Episodic fluctuations in larval supply. Science 283:1528–1530.

Sugihara G. and May R. 1990. Nonlinear forecasting as a way of distinguishing chaos from measurement error in time series. Nature, 344:734–741.

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Sugihara G., May R., Ye H., Hsieh C., Deyle E., Fogarty M., Munch S., 2012. Detecting Causality in Complex Ecosystems. Science 338:496-500.

Takens, F. Detecting strange attractors in turbulence. Lect. Notes Math. 898, 366–381 (1981).

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