

pyEDM Version 0.1.3 June 21, 2019

pyEDM is a Python package interface to the cppEDM C++ library of empirical dynamic modeling (EDM) algorithms. It is loaded within Python by `import EDM` and returns Pandas DataFrame objects.

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Introduction

pyEDM is a Python interface to the C++ library cppEDM. Input and output objects are based on Pandas DataFrame objects. Core algorithms are listed in table 1.

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

Convenience functions to prepare and evaluate data are listed in table 2.

| Function | Purpose | Parameter Range |
|---------------------------------|---|--|
| <code>Embed()</code> | Timeseries delay dimensional embedding | User defined |
| <code>MakeBlock()</code> | Timeseries delay dimensional embedding | User defined |
| <code>EmbedDimension()</code> | Evaluate prediction skill vs. embedding dimension | $E = [1, 10]$ |
| <code>PredictInterval()</code> | Evaluate prediction skill vs. forecast interval | $T_p = [1, 10]$ |
| <code>PredictNonlinear()</code> | Evaluate prediction skill vs. SMap nonlinear localisation | $\theta = 0.01, 0.1, 0.3, 0.5, 0.75, 1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9$ |
| <code>ComputeError()</code> | Pearson ρ , RMSE, MAE | |
| <code>Examples()</code> | Example function calls and plots | |

Installation

Unfortunately, we do not have the resources to provide pre-built binary distributions for the various computer platforms. The user is required to first build the cppEDM library on their machine, and then install the Python package using pip. On OSX and Linux this requires gcc, on Windows, Microsoft Visual Studio Compiler (MSVC) which can be obtained from Build Tools for Visual Studio 2019. Only the Windows SDK is needed.

Note that the Eigen C++ Template Library is required to build cppEDM. It is assumed that the Eigen directory is available in the compiler INCLUDE path. If not, you can add the directory to the CFLAGS -I option in the makefile, appropriately define the INCLUDE environment variable, or, override the make command line with CFLAGS= to specify the location.

OSX and Linux

1) Download pyEDM: git clone <https://github.com/SugiharaLab/pyEDM>

2) Build cppEDM library:

```
cd pyEDM/cppEDM/src
```

```
make CFLAGS="-std=c++11 -DCCM_THREADED -DMULTIVIEW_VALUES_OVERLOAD -O3 -fPIC"
```

3) Build and install package:

```
cd ../../
```

```
python -m pip install . --user
```

Windows

1) Download pyEDM: git clone <https://github.com/SugiharaLab/pyEDM>

2) Build cppEDM library:

```
cd pyEDM/cppEDM/src
```

```
nmake /f makefile.windows
```

3) Copy the cppEDM/lib/libEDM.a into pyEDM/lib.

4) Build and install package:

```
cd ../../
```

```
python -m pip install . --user
```

Usage

```
>>> import EDM
>>> EDM.Examples()
```

Parameters

API parameter names and purpose are listed in table 3.

| Parameter | Type | Default | Purpose |
|-----------------|------------------|---------|--|
| pathIn | string | "./" | Input data file path |
| dataFile | string | " " | Data file name |
| dataFrame | Pandas DataFrame | None | Input DataFrame |
| pathOut | string | "./" | Output file path |
| predictFile | string | " " | Prediction output file |
| lib | string | " " | library start : stop row indices |
| pred | string | " " | prediction start : stop row indices |
| E | int | 0 | Data dimension |
| Tp | int | 0 | Prediction interval |
| knn | int | 0 | Number nearest neighbors |
| tau | int | 1 | Embedding delay |
| theta | float | 0 | SMap localisation |
| exclusionRadius | int | 0 | Prediction vector exclusion radius |
| columns | string | " " | Column names or indices for prediction |
| target | string | " " | Target library column name or index |
| embedded | bool | false | Is data an embedding? |
| const_pred | bool | false | Include non projected forecast data |
| verbose | bool | false | Echo messages |
| smapFile | string | " " | SMap coefficient output file |
| libSizes_str | string | " " | CCM library sizes |
| sample | int | 0 | CCM number of random samples |
| random | bool | true | CCM use random samples? |
| seed | unsigned | 0 | RNG seed, 0 = random seed |

Application Programming Interface (API)

Embed

Create a data block of Takens (1981) time-delay embedding from each of the columns in the csv file or dataframe. The columns parameter can be a list of column names, or a list of column indices. If columns is a list of indices, then column names are created as V1, V2...

Note: The returned DataFrame will have $\tau \cdot (E - 1)$ fewer rows than the input data from the removal of partial vectors as a result of the embedding.

Note: The returned DataFrame will not have the time column.

```
//-----  
//  
//-----  
DataFrame Embed ( path      = "",  
                  dataFile  = "",  
                  dataframe = None,  
                  E         = 0,  
                  tau       = 0,  
                  columns   = "",  
                  verbose   = false )  
  
//-----  
//  
//-----  
DataFrame MakeBlock ( dataframe,  
                    E,  
                    tau,  
                    columnNames,  
                    verbose )
```

Simplex

Simplex projection of the input data file or DataFrame. The returned DataFrame has 3 columns "Time", "Observations", "Predictions". nan values are inserted where there is no observation or prediction. See the Parameters table for parameter definitions.

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

```
//-----  
//  
//-----  
DataFrame Simplex( pathIn      = "./data/",  
                   dataFile    = "",  
                   dataframe    = None,  
                   pathOut     = "./",  
                   predictFile  = "",  
                   lib         = "",  
                   pred        = "",  
                   E           = 0,  
                   Tp          = 1,  
                   knn         = 0,  
                   tau         = 1,  
                   exclusionRadius = 0,  
                   columns     = "",  
                   target      = "",  
                   embedded     = false,  
                   const_pred  = false,  
                   verbose     = true )
```

SMap

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

SMap() returns a dict with two DataFrames:

```
dict { predictions : DataFrame,  
        coefficients : DataFrame  
}
```

The predictions DataFrame has 3 columns "Time", "Observations", "Predictions". nan values are inserted where there is no observation or prediction. If predictFile is provided the predictions will be written to it in csv format.

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.

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 smapFile is provided the coefficients will be written to it in csv format.

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

```
//-----  
//  
//-----  
dict SMap( pathIn      = "./data/",  
           dataFile    = "",  
           dataframe    = None,  
           pathOut     = "./",  
           predictFile  = "",  
           lib         = "",  
           pred        = "",  
           E           = 0,  
           Tp          = 1,  
           knn         = 0,  
           tau         = 1,  
           theta       = 0,  
           exclusionRadius = 0,  
           columns     = "",  
           target      = "",  
           smapFile    = "",  
           derivatives  = "", // Not implemented  
           embedded    = false,  
           const_pred   = false,  
           verbose     = true )
```

CCM

Convergent cross mapping via Simplex of the first vector specified in `columns` against `target`. The data cannot be multivariable, the first vector in `columns` is time-delay embedded to dimension `E`. See the Parameters table for parameter definitions.

The returned `DataFrame` has 3 columns. The first column is "LibSize", the second and third columns are Pearson correlation coefficients for "column : target" and "target : column" cross mapping.

`libSizes` specifies a string with "start stop increment" row values, i.e. "10 80 10" will evaluate library sizes from 10 to 80 in increments of 10.

If `random` is `true`, sample observations are randomly selected from the subset of each library size. If `seed=0`, then a random seed is generated for the random number generator. Otherwise, `seed` is used to initialise the random number generator.

If `random` is `false`, `sample` is ignored and contiguous library rows up to the current library size are used.

Note: Cross mappings are performed between `column : target`, and `target : column`. The default is to do this in separate threads. Threading can be disabled in the makefile by removing `-DCCM_THREADED`.

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

```
//-----  
//  
//-----  
DataFrame CCM( pathIn      = "./data/",  
               dataFile    = "",  
               dataframe    = None,  
               pathOut     = "./",  
               predictFile  = "",  
               E            = 0,  
               Tp          = 0,  
               knn          = 0,  
               tau          = 1,  
               columns      = "",  
               target       = "",  
               libSizes     = "",  
               sample       = 0,  
               random       = true,  
               seed         = 0, // seed=0: use RNG  
               verbose      = true );
```


Multiview

Multiview embedding and forecasting of the input data file or DataFrame. See the Parameters table for parameter definitions.

`Multiview()` returns a dict:

```
dict { Combo_rho    : DataFrame,  
        Predictions : DataFrame  
}
```

The Predictions DataFrame has 3 columns "Time", "Observations", "Predictions". nan values are inserted where there is no observation or prediction. If predictFile is provided the Predictions will be written to it in csv format.

The Combo_rho DataFrame will have E+3 columns. The first E columns are the the column indices in the input data DataFrame that are embedded and applied to Simplex prediction. The last three columns are "rho", "MAE", "RMSE" corresponding to the prediction Pearson correlation, maximum absolute error and root mean square error.

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

If multiview is not specified it is set to \sqrt{C} where C is the number of E-dimensional combinations out of all available data vectors.

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

```
//-----  
//  
//-----  
dict Multiview( pathIn      = "./",  
                dataFile   = "",  
                dataframe   = None,  
                pathOut    = "./",  
                predictFile = "",  
                lib        = "",  
                pred       = "",  
                E          = 0,  
                Tp         = 1,  
                knn        = 0,  
                tau        = 1,  
                columns     = "",  
                target      = "",  
                multiview   = 0,  
                verbose     = false,  
                nThreads   = 4 )
```

EmbedDimension

Evaluate Simplex prediction skill for embedding dimensions from 1 to 10. The returned `DataFrame` has columns "E" and "rho". See the Parameters table for parameter definitions.

Note: `nThreads` defines the number of worker threads for the 10 embeddings. The maximum number of threads is 10.

```
//-----  
//  
//-----  
DataFrame EmbedDimension( pathIn      = "./data/",  
                          dataFile    = "",  
                          dataframe    = None,  
                          pathOut     = "./",  
                          predictFile = "",  
                          lib         = "",  
                          pred        = "",  
                          Tp          = 1,  
                          tau         = 1,  
                          columns     = "",  
                          target      = "",  
                          embedded    = false,  
                          verbose     = true,  
                          nThreads    = 4 )
```

PredictInterval

Evaluate Simplex prediction skill for forecast intervals from 1 to 10. The returned DataFrame has columns "Tp" and "rho". See the Parameters table for parameter definitions.

Note: nThreads defines the number of worker threads for the 10 prediction interval forecasts. The maximum number of threads is 10.

```
//-----  
// Overload 1: Explicit data file path/name  
//-----  
DataFrame PredictInterval( pathIn      = "./data/",  
                           dataFile    = "",  
                           dataframe    = None,  
                           pathOut     = "./",  
                           predictFile = "",  
                           lib         = "",  
                           pred        = "",  
                           E           = 0,  
                           tau         = 1,  
                           columns     = "",  
                           target      = "",  
                           embedded    = false,  
                           verbose     = true,  
                           nThreads    = 4 );
```

PredictNonlinear

Evaluate SMap prediction skill for localisation parameter θ from 0.01 to 9. The returned DataFrame has columns "theta" and "rho". See the Parameters table for parameter definitions.

Note: nThreads defines the number of worker threads for the 15 θ value forecasts.

```
//-----  
//  
//-----  
DataFrame PredictNonlinear( pathIn      = "./data/",  
                             dataFile   = "",  
                             dataframe   = None,  
                             pathOut    = "./",  
                             predictFile = "",  
                             lib        = "",  
                             pred       = "",  
                             E          = 0,  
                             Tp         = 1,  
                             tau        = 1,  
                             columns    = "",  
                             target     = "",  
                             embedded    = false,  
                             verbose    = true,  
                             nThreads   = 4 );
```

ComputeError

Compute Pearson correlation coefficient, maximum absolute error (MAE) and root mean square error (RMSE) between two vectors.

`ComputeError()` returns a dict:

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

```
//-----  
//-----  
dict ComputeError( obsIn, predIn )
```

Application Notes

All data input files are assumed to be in csv format. The files are assumed to have a single line header with column names. If column names are not detected in the header line, then column names are created as V1, V2... **It is required that the first column be a vector of times or time indices.**

`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 then not correspond to the intended dimensions in the matrix inversion and prediction reconstruction. In this case, use the `embedded` parameter set to `true` so that the columns selected correspond to the proper dimension.

Examples

```
df = EmbedDimension( "./data/", "TentMap_rEDM.csv", None, "./", "",
                    "1 100", "201 500", 1, 1,
                    "TentMap", "", False, False, 4 )

df = PredictInterval( "./data/", "TentMap_rEDM.csv", None, "./", "",
                    "1 100", "201 500", 2, 1,
                    "TentMap", "", False, False, 4 )

df = PredictNonlinear( "./data/", "TentMapNoise_rEDM.csv", None, "./", "",
                    "1 100", "201 500", 2, 1, 1,
                    "TentMap", "", False, False, 4 )

df = Simplex( "./data/", "block_3sp.csv", None, "./", "",
              "1 99", "100 198", 3, 1, 0, 1,
              "x_t y_t z_t", "x_t", True, True, True )

df = Simplex( "./data/", "block_3sp.csv", None, "./", "",
              "1 99", "100 195", 3, 1, 0, 1,
              "x_t", "x_t", False, True, True )

M = Multiview( "./data/", "block_3sp.csv", None, "./", "",
              "1 100", "101 198", 3, 1, 0, 1,
              "x_t y_t z_t", "x_t", 0, False, 4, True )

S = SMap( "./data/", "circle.csv", None, "./", "",
          "1 100", "101 198", 2, 1, 0, 1, 4,
          "x y", "x", "", "", True, True, True )

df = CCM( "./data/", "sardine_anchovy_sst.csv", None, "./", "",
          3, 0, 0, 1, "anchovy", "np_sst",
          "10 80 10", 100, True, 0, True, 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.

Sugihara G. 1994. Nonlinear forecasting for the classification of natural time series. *Philosophical Transactions: Physical Sciences and Engineering*, 348 (1688) : 477–495.

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).

Ye H., and G. Sugihara, 2016. Information leverage in interconnected ecosystems: Overcoming the curse of dimensionality. *Science* 353:922–925.