cppEDM Version 1.14.3 July 5, 2023

cppEDM is a C++ implementation of empirical dynamic modeling (EDM) algorithms. It is designed as an application programming interface (API) to functions in the libEDM.a library. A Python interface is provided in PyPI package <u>pyEDM</u>, an R interface in CRAN package <u>rEDM</u>. A Jupyter notebook GUI front-end is provided in <u>jpyEDM</u>.

Table of Contents

Introduction	2
Installation	
Class Objects	3
DataFrame	
Parameters	
Application Programming Interface (API)	6
Embed	
Simplex	7
SMap	
CCM	
Multiview	15
EmbedDimension	17
PredictInterval	18
PredictNonlinear	
ComputeError	
Application Notes	
Example Application	
Code Notes	
References	23

University of California at San Diego Scripps Institution of Oceanography Sugihara Lab

Joseph Park, Cameron Smith

Introduction

<u>cppEDM</u> is a C++ implementation of empirical dynamic modeling (<u>EDM</u>) algorithms. Primary algorithms are listed in table 1. The core code is an object oriented implementation supporting application programming interface (API) functions accepting parameters and returning data objects. EDM functions are accessed from a user-compiled library created from C++ source files and a unix-like compiler supporting the C++11 standard. cppEDM has Python and R interfaces implemented in the <u>pvEDM</u> and <u>rEDM</u> packages.

Algorithm	API Interface	Reference
Simplex projection	Simplex()	Sugihara and May (1990)
Sequential Locally Weighted Global Linear Maps (S-map)	SMap()	Sugihara (1994)
Predictions from multivariate embeddings	<pre>Simplex(), SMap()</pre>	Dixon et. al. (1999)
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.

Function	Purpose	Parameter Range
Embed()	Timeseries delay dimensional embedding	User defined
<pre>EmbedDimension()</pre>	Evaluate prediction skill vs. embedding dimension	E = [1, 10]
<pre>PredictInterval()</pre>	Evaluate prediction skill vs. forecast interval	Tp = [1, 10]
PredictNonlinear()	Evaluate prediction skill vs. SMap nonlinear localisation	θ = 0.01, 0.1, 0.3, 0.5, 0.75, 1, 1.5, 2, 3, 4, 5, 6, 7, 8, 9
ComputeError()	Pearson correlation, MAE, RMSE	

Installation

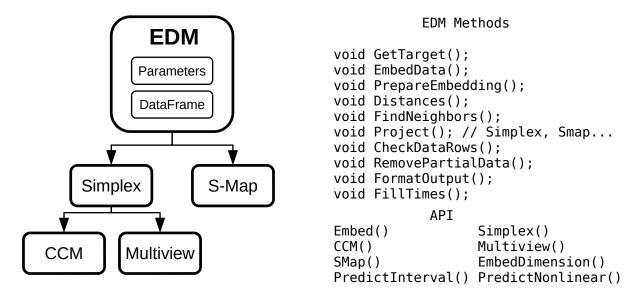
cppEDM is available at github.com/SugiharaLab/cppEDM.

cppEDM requires a C++11 standard compiler, and the LAPACK library. The libEDM.a library can be built by running "make" in the cppEDM/src/ directory. This copies libEDM.a into the cppEDM/lib/ directory, where it can be linked to user applications.

Once libEDM.a is built, there are a series of test applications in the cppEDM/tests/ directory. The applications can be built with the "make" command, and executed at the command line. API examples can also be found in cppEDM/etc/Test.cc.

Class Objects

cppEDM is a C++ Object Oriented (OO) implementation. The primary data class is EDM, from which the algorithm classes are derived. The class hierarchy is:



Two C++ class objects are used for data access and parameter coordination, the DataFrame and Parameters classes, described below.

DataFrame

The DataFrame class is the fundamental data object of cppEDM. It stores data in a contiguous block of memory using the C++ valarray type in a row-major format.

A DataFrame can be initialised with data from a csv file by calling the DataFrame constructor with path and fileName parameters. Data input files are assumed to be in csv format. The files are required to have a single line header with column names.

It is assumed that the first column of the csv file is a vector of times or time indices for each observation (row). All subsequent columns are expected to be numeric. However, a DataFrame can be created with the noTime = true parameter to read in numeric data with no time in the first column. Such data frames should not be passed to prediction functions.

The WriteData(path, file) class method can be called explicitly to write data to a csv format file. If the DataFrame does not have column names, then column names are created as V1, V2...

Primary DataFrame access functions are listed in table 3.

DataFrame Method	Parameters	Type	Purpose
(row, column)	size_t row size_t column	double or int	Access data element
DataFrame(path, file)	string path string fileName	DataFrame <double></double>	Create DataFrame from csv file
WriteData(path, file)	string outputFilePath string outputFileName		Write DataFrame to file
<pre>Elements()</pre>		valarray	Access data valarray
NColumns()		size_t	Get number of columns
NRows ()		size_t	Get number of rows
size()		size_t	Get number of elements
ColumnNames()		vector< string >	Access column names
ColumnNameToIndex()		<pre>map<string, size_t=""></string,></pre>	Access column name to index map
MaxRowPrint()		size_t	Access maximum number of rows to ostream
Column(col)	size_t col	valarray	Get data vector at column
Row(row)	size_t row	valarray	Get data vector at row
VectorColumnName(column)	string column	valarray	Get data vector at column with name
ColumnMajorData()		valarray	Elements() in column major format.
<pre>DataFrameFromColumnIndex (columns)</pre>	vector <size_t> columns</size_t>	DataFrame <double></double>	Get DataFrame subset from column indices
<pre>DataFrameFromColumnNames (columns)</pre>	vector <string> columns</string>	DataFrame <double></double>	Get DataFrame subset from column names
<pre>DataFrameFromRowIndex (rows)</pre>	vector <size_t> rows</size_t>	DataFrame <double></double>	Get DataFrame subset from row indices
WriteRow(row, array)	<pre>size_t row std::valarray<t> array</t></pre>		Write valarray to row
WriteColumn(col, array)	size_t col valarray <t> array</t>		Write valarray to column

Parameters

The Parameters class is used to store and access API function parameters in a unified object. Generally this is an internal object that does not need to be instantiated, accessed or dynamically modified. API parameter names and purpose are listed in table 4.

Parameter	Type	Default	Purpose
pathIn	string	"./"	Input data file path
dataFile	string	и и	Data file name
pathOut	string	"./"	Output file path
predictFile	string	н н	Prediction output file
smapFile	string	шш	SMap coefficient output file
lib	string	шш	library start : stop row indices
pred	string	шш	prediction start : stop row indices
E	int	0	Embedding dimension
Тр	int	0 or 1	Prediction interval (rows)
knn	int	0	Number nearest neighbors
tau	int	-1	Embedding offset (time series rows)
theta	double	0	SMap localisation
exclusionRadius	int	0	Prediction vector exclusion row radius
columns	string	шш	Column names or indices for prediction
target	string	шш	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
validLib	vector <bool></bool>	[]	Conditional Embedding (CE)
generateSteps	int	0	Simplex, SMap feedback prediction
generateLibrary	bool	false	Increment EDM library with feedback
parameterList	bool	false	Return Parameters map
multiview	int	0	Number of ensembles, $0 = \text{sqrt}(N)$
D	int	0	Multiview dimension
trainLib	bool	true	Multiview use lib as training library
excludeTarget	bool	false	Multiview exlcude target from combos
libSizes	string	н н	CCM library sizes
sample	int	0	CCM number of random samples
random	bool	true	CCM use random samples?
replacement	bool	false	CCM sample with replacement?
includeData	bool	false	CCM include all projections in return
seed	unsigned	0	CCM 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 | * (E-1) fewer rows than the input data from the removal of partial vectors as a result of the embedding.

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

```
//-----
// Overload 1: Explicit data file path/name
//-----
DataFrame< double > Embed ( std::string path = "",
                  std::string dataFile = ""
                         \mathsf{E} \qquad = 0,
                  int
                         tau = -1,
                  int
                  std::string columns = "",
                  bool verbose = false );
//-----
// Overload 2: DataFrame provided
//-----
DataFrame< double > Embed ( DataFrame< double > dataFrame,
                  int E = 0,
                  int
                              tau
                              columns = "".
                  std::string
                  bool
                               verbose = false );
//-----
// Called from Embed to create the time-delay embedding
DataFrame< double > MakeBlock ( DataFrame< double >
                                     dataFrame,
                    int
                                     Ε,
                    int
                                     tau,
                    std::vector<std::string> columnNames,
                                     deletePartial = false );
```

Simplex

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

Simplex() returns a SimplexValues structure:

The predictions DataFrame has 3 columns "Time", "Observations", "Predictions". nan values are inserted where there is no observation or prediction. The parameterMap returns a map of parameters used in the predictions if parameterList = true.

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 time offset tau. If embedded is true the data columns are assumed to be a multivariable data block.

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 ± 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 generateSteps > 0, then Simplex and SMap operate in feedback generative mode. The values of pred are over-riden to start at the end of the data. At each step one prediction is made, added to the columns data, a new time-delay embedded is created, and the cycle repeated for generateSteps. Feedback generation only operates on a univariate time series that is time-delay embedded. The columns and target variables must be the same. If generateLibrary is false the state-space library is not expanded as predictions are generated, it is static. If generateLibrary is true the state-space library has the generated prediction added to the library at each step.

If parameterList = true, then parameterMap is populated.

```
// Overload 1: Explicit data file path/name
//-----
SimplexValues Simplex( std::string pathIn = "./data/", std::string dataFile = "",
                   std::string pathOut
                   std::string predictFile
                   std::string lib
                   std::string pred
                             Е
                   int
                   int
                             Tp
                                           = 0,
                   int
                             knn
                   int
                             tau
                                           = -1.
                   int
                             exclusionRadius = 0,
                   std::string columns = ""
                                          = ""
                   std::string target
                   bool
                             embedded
                                         = false,
                             const_pred = = false,
                   bool
                                          true,
                   bool
                             verbose
                   std::vector<bool> validLib = std::vector<bool>(),
                             generateSteps = 0,
                   bool
                             generateLibrary = false,
                   bool
                             parameterList = false );
//-----
// Overload 2: DataFrame reference provided
//-----
SimplexValues Simplex( DataFrame< double > & dataFrameIn,
                   std::string pathOut = "./",
                                          = ""
                   std::string predictFile
                                          = ""
                   std::string lib
                   std::string pred
                   int
                             Ε
                                          = 0,
                   int
                             Tp
                   int
                             knn
                                           = 0.
                                           = -1,
                   int
                             tau
                             exclusionRadius = 0.
                   int
                   std::string columns = ""
                                          = "".
                   std::string target
                             embedded
                                          = false,
                   bool
                             embedded
const_pred
                                         = false,
                   bool
                                          = true,
                   bool
                             verbose
                   std::vector<bool> validLib = std::vector<bool>(),
                             generateSteps = 0,
                   int
                   bool
                             generateLibrary = false,
                   bool
                             parameterList = false );
```

SMap

SMap projection of the input data file or DataFrame. See the Parameters table for parameter definitions. If nan are detected in the columns or target, those rows are removed prior to any time-delay embedding. This may violate the presumes of Takens theorem.

SMap() returns a SMapValues structure:

```
struct SMapValues {
    DataFrame< double > predictions;
    DataFrame< double > coefficients;
    std::map< std::string, std::string > parameterMap;
};
```

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 csy 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. The first column "C0" is the bias term, following coefficients are ∂ columns[i] / ∂ target.

The parameterMap returns a map of parameters used in the predictions if parameterList = true.

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 offset 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 csy format.

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.

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 ± 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.

The default solver for the SMap coefficient matrix is the LAPACK SVD function dgelss().

If generateSteps > 0, then Simplex and SMap operate in feedback generative mode. The values of pred are over-riden to start at the end of the data. At each step one prediction is made, added to the columns data, a new time-delay embedded is created, and the cycle repeated for generateSteps. Feedback generation only operates on a univariate time series that is time-delay embedded. The columns and target variables must be the same. If generateLibrary is false the state-space library is not expanded as predictions are generated, it is static. If generateLibrary is true the state-space library has the generated prediction added to the library at each step.

If parameterList = true, parameterMap is populated.

```
SMap
```

```
//-----
// Overload 1: Explicit data file path/name
//-----
SMapValues SMap( std::string pathIn = "./data/",
                                         = "",
                std::string dataFile
                std::string pathOut
                std::string predictFile = ""
std::string lib = ""
                                          = ""
                std::string lib
                                          = ""
                std::string pred
                                          = 0,
                           Е
                int
                int
                           Τp
                                          = 1,
                int
                           knn
                                          = 0.
                int
                           tau
                                          = -1.
                                          = 0,
                double
                           theta
                           exclusionRadius = 0,
                int
                                          = ""
                std::string columns
                                          = ""
               std::string smapFile = "",
std::string smapFile = "",
std::string derivatives = "",
bool embedded = false,
bool const_pred = false,
bool verbose = true.
                std::string target
                                                 // Not implemented
                std::vector<bool> validLib = std::vector<bool>(),
                           generateSteps = 0,
                int
                           generateLibrary = false,
                bool
                           parameterList = false );
                bool
//----
// Overload 2: DataFrame reference provided
//-----
SMapValues SMap( DataFrame< double > &dataFrameIn,
                std::string pathOut = "./"
                                        = ""
                std::string predictFile
                                          = ""
                std::string lib
                                         = ""
                std::string pred
                           Е
                                          = 0,
                int
                           Tp
                                          = 1,
                int
                int
                           knn
                                          = 0,
                           tau
                                          = -1.
                int
                double
                           theta
                                          = 0,
                           exclusionRadius = 0,
                int
                std::string columns = ""
                                          = ""
                std::string target
               std::string target - ,
std::string smapFile = "",
std::string derivatives = "",
bool embedded = false,
                                                   // Not implemented
                bool
                           const pred
                                          = false,
                bool
                           verbose
                                          = true,
                std::vector<bool> validLib = std::vector<bool>(),
                int
                           generateSteps = 0,
                bool
                           generateLibrary = false,
                           parameterList = false );
                bool
```

```
SMap
//----
            ------
// Overload 3: Data path/file with external solver object, init to default SVD
//-----
SMapValues SMap( std::string pathIn = "./data/",
                                     = "",
              std::string dataFile
                                      = "./"
              std::string pathOut
                                      = ""
              std::string predictFile
                                      = ""
              std::string lib
                                     = ""
              std::string pred
                         Е
                                      = 0,
              int
              int
                         Тp
                                       = 1.
                                       = 0,
              int
                         knn
              int
                         tau
                                       = -1.
                         theta
              double
                                       = 0,
                         exclusionRadius = 0,
              int
              std::string columns = ""
                                      = ""
              std::string target
                                     = ""
              std::string smapFile
              std::string derivatives = ",
                                              // Not implemented
              std::valarray<double> (*solver)(DataFrame < double >,
                                       std::valarray < double >) = &SVD,
              bool
                         embedded
                                       = false,
              bool
                         const predict = false,
              bool
                         verbose
                                     = true,
              std::vector<bool> validLib = std::vector<bool>(),
                         generateSteps = 0,
              bool
                         generateLibrary = false,
              bool
                         parameterList = false );
//-----
// Overload 4: DataFrame with external solver object, init to default SVD
//-----
SMapValues SMap( DataFrame< double > &dataFrameIn,
              std::string pathOut = "./"
                                      = ""
              std::string predictFile
                                    = ""
              std::string lib
                                      = ""
              std::string pred
              int
                        Ε
                                       = 0,
                                      = 1,
              int
                         Tp
              int
                         knn
                                       = 0,
                        tau
              int
                                       = -1.
              \begin{array}{lll} \mbox{double} & \mbox{theta} & = \mbox{0,} \\ \mbox{int} & \mbox{exclusionRadius} & = \mbox{0,} \\ \end{array}
              std::string columns = ""
                                      = ""
              std::string target
                                      = ""
              std::string smapFile
              std::string derivatives = "",
                                              // Not implemented
              std::valarray<double> (*solver)(DataFrame < double >,
                                       std::valarray < double >) = &SVD,
              bool
                         embedded
                                       = false,
              bool
                         const predict = false,
              bool
                         verbose
                                       = true,
              std::vector<bool> validLib = std::vector<bool>(),
                         generateSteps = 0,
              int
                         generateLibrary = false,
              bool
              bool
                         parameterList = false );
```

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, not an embedding.

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 threads. Threading can be disabled in the makefile by removing -DCCM_THREADED.

Note: The entire prediction vector is used in the Simplex prediction at each library subset size. See the Parameters table for parameter definitions.

CCM() returns a CCMValues structure:

CCMValues::LibStats 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.

If the includeData parameter is true, then the CrossMapValues structures CrossMap1 and CrossMap2 in CCMValues are populated with the DataFrame PredictStats and list of DataFrames Predictions. LibStats is used for internal storage, and is empty upon return.

Parameters

The libSizes parameter is a string of whitespace or comma separated library sizes. If the string has 3 values, and, if the third value is less than the second value, then 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 random is true, sample observations are radomly selected from the subset of each library size. If replacement is true, observations are selected with replacement. If seed=0 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 this is not Convergent Cross Mapping (CCM).

```
// Overload 1: Explicit data file path/name
//-----
            = -1,
            std::string columns = ""
                                 = ""
            std::string target
// Overload 2: DataFrame reference provided
//-----
CCMValues CCM( DataFrame< double > &dataFrameIn,
            std::string pathOut = "./",
            std::string predictFile = "",
int E = 0,
            std::string columns = ""
            std::string columns = "",
std::string target = "",
std::string libSizes = "",
int sample = 0,
bool random = true,
bool replacement = false,
unsigned seed = 0,
bool embedded = false,
bool includeData = false,
bool verbose = true );
                                          // seed=0: use RNG
```

Multiview

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

Multiview() returns a MultiviewValues structure:

```
struct MultiviewValues {
    DataFrame< double > ComboRho;
    DataFrame< double > Predictions;
    std::map< std::string, std::vector< std::string > > ColumnNames;
    std::map< std::string, std::string > parameterMap;
};
```

The ComboRho DataFrame has D+3 columns. The first D columns are the the column indices in the input DataFrame embedding (not the input DataFrame) and are applied to multivariate Simplex predictions. The last three columns are "rho", "MAE", "RMSE" corresponding to the prediction Pearson correlation, maximum absolute error and root mean square error.

ColumnNames is a map of string vectors listing the multiview embedding column names of the input DataFrame embedding.

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

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.

```
// Overload 1: Explicit data file path/name
//-----
MultiviewValues Multiview( std::string pathIn = "./", std::string dataFile = "", std::string pathOut = "./",
                           std::string predictFile
                           std::string lib
                           std::string pred
                           int
                                  D
                                      Ε
                           int
                           int
                                       Τp
                                                       = 1,
                           int
                                      knn
                                                       = 0,
                                                       = -1,
                           int
                                   tau = -1,
ing columns = "",
ing target = "",
multiview = 0,
                                      tau
                           std::string columns
                           std::string target
                           int
                           int
                                       exclusionRadius = 0,
                           bool
                           bool trainLib = true,
bool excludeTarget = false,
bool parameterList = false,
bool verbose = false,
unsigned nThreads = 4 );
                                      trainLib = true,
// Overload 2: DataFrame provided
//-----
MultiviewValues Multiview( DataFrame< double >,
                           std::string pathOut
                           std::string predictFile
std::string lib
                           std::string lib
                           std::string pred
                           int
                                       D
                                                       = 0,
                                       Ε
                                                       = 1,
                           int
                           int
                                       Tp
                                                       = 1.
                                                       = 0,
                           int
                                      knn
                           int cau
std::string columns
                                                       = ""
                           std::string target
                                 multiview
                                                      = 0,
                           int
                                       exclusionRadius = 0,
                           int
                           bool
                                       trainLib
                                                = true,
                           bool
                                     excludeTarget = false,
                                       parameterList = false,
                           bool
                                       verbose = false,
nThreads = 4);
                           bool
                           unsigned nThreads
```

EmbedDimension

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

```
// Overload 1: Explicit data file path/name
//-----
DataFrame<double> EmbedDimension( std::string pathIn
                         std::string pred
                              maxE
Tp
                         int
                         int
                         int
                                  tau
                             exclusionRadius = 0,
                         int
                         std::string columns = ""
                                             = ""
                         std::string target
                                embedded = false,
verbose = true.
                         bool
                         bool
                                 verbose
                                              = true,
                         std::vector<bool> validLib =
                                      std::vector<bool>(),
                         unsigned nThreads
                                              = 4 ):
//-----
// Overload 2: DataFrame reference provided
//-----
DataFrame<double> EmbedDimension( DataFrame< double > &dataFrameIn,
                         std::string pathOut = "./"
                         std::string predictFile
                         std::string lib
                                            = ""
                         std::string pred
                               maxE
                         int
                         int
                                  Tp
                         int
                                  tau
                         int
                                  exclusionRadius = 0,
                         std::string columns = ""
                              embedded = "",

verbose = true
                         std::string target
                         bool
                         ustd::vector<bool> validLib =
                                       std::vector<bool>(),
                         nsigned
                                 nThreads
                                              = 4 );
```

PredictInterval

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

```
// Overload 1: Explicit data file path/name
 //----
DataFrame<double> PredictInterval( std::string pathIn std::string dataFile std::string pathOut std::string predictFile std::string lib st
                                                                                              E = 0,
tau = -1
exclusionRadius = 0,
                                                                                               int
                                                                                                                                               = -1,
                                                                                              int
                                                                                              int
                                                                                              std::string columns = ""
                                                                                                                 std::string target
                                                                                              bool
                                                                                              bool
                                                                                               std::vector<bool> validLib =
                                                                                                                                               std::vector<bool>(),
                                                                                              unsigned nThreads = 4);
 //-----
 // Overload 2: DataFrame reference provided
 //-----
 DataFrame<double> PredictInterval( DataFrame< double > &dataFrameIn,
                                                                                              std::string pathOut = "./"
                                                                                              std::string pred
                                                                                              int maxTp
                                                                                                                                                                        = 10.
                                                                                                                          Е
                                                                                               int
                                                                                              int tau = -1
int exclusionRadius = 0,
                                                                                               std::string columns = ""
                                                                                              std::vector<bool>(),
                                                                                              unsigned
                                                                                                                               nThreads
                                                                                                                                                                        = 4 );
```

PredictNonlinear

Evaluate SMap prediction skill for localisation parameters θ specified in the string theta. Default values of theta are "0.01 0.1 0.3 0.5 0.75 1 1.5 2 3 4 5 6 7 8 9". Default knn (0) sets to size of the library. Smaller knn values can be specified.

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 \theta value forecasts.
//-----
// Overload 1: Explicit data file path/name
//-----
std::string dataFile = ""

std::string pathOut = ".,

std::string predictFile = ""
                          std::string lib
                          std::string pred
std::string theta
                          int E
                                             = 1,
                          int
                                 Tp
                         = -1.
                          std::string columns = ""
                              embedded = false,
verbose = true
                          std::string target
                          bool
                          bool
                          std::vector<bool> validLib =
                                       std::vector<bool>(),
                          unsigned nThreads
//-----
// Overload 2: DataFrame reference provided
//-----
DataFrame<double> PredictNonlinear( DataFrame< double > &dataFrameIn,
                          std::string pathOut = "./",
                          std::string predictFile
                          std::string lib
                          std::string pred
                          std::string theta
                                  Е
                                             = 0,
                          int
                                  Тp
                                              = 1,
                          int
                         int
                                  knn
                                             = 0,
                                              = -1,
                          int
                                  tau
                          int exclusionRadius = 0,
                          std::string columns = ""
                                             = ""
                          std::string target
                                  embedded = false,
verbose = true,
                          bool
                          bool
                          std::vector<bool> validLib =
                                        std::vector<bool>(),
                          unsigned nThreads = 4);
```

ComputeError

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

ComputeError() returns a VectorError struct:

Application Notes

All data input files are assumed to be in csv format. The files are required to have a single line header with column names.

It is assumed that the first column of the csv file is a vector of times or time indices for each observation (row). All subsequent columns are expected to be numeric. However, a DataFrame can be created with the noTime = true parameter to read in numeric data with no time in the first column. Such data frames should not be passed to prediction functions.

SMap () should be called with DataFrame that have columns explicitly corresponding to dimensions E. Subsequently, 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. In this case, use the embedded parameter set to true so that the columns selected correspond to the proper dimension.

See etc/Notes for details regarding the building an application (etc/Test.cc) on Windows.

See etc/Notes for an explanation of differences between Simplex() and CCM() default embeddings, and the effect this has on predictions.

Example Application

This application is assumed to be located in the etc/ directory. Otherwise, adust the -I and -L compiler flags and the pathIn argument accordingly. The file etc/Test.cc shows sample invocations for several API functions.

```
// g++ TestApp.cc -o TestApp -g -I../src -L../lib -lstdc++ -lEDM -llapack
#include "API.h"
int main( int argc, char *argv[] ) {
   try {
       //-----
       // embedded = false : Simplex embeds all columns to E = 3
       //-----
       DataFrame<double> dataFrame =
                    "../data/", // pathIn
"block_3sp.csv", // dataFile
"./", // pathOut
           Simplex( "../data/",
                    "Block3sp_E3.csv", // predictFile
                    "1 100",
                                       // lib
                    "101 195",
                                       // pred
                                       // E
                     3,
                     1,
                                       // Tp
                                       // knn
                     0.
                     -1,
                                       // tau
                                      // exclusionRadius
                    "x_t y_t z_t", // columns
                    "x_t",
                                      // target
                                      // embedded
                    false,
                    false.
                                      // const predict
                    true );
                                       // verbose
       dataFrame.MaxRowPrint() = 12; // Set number of rows to print
       std::cout << dataFrame;</pre>
       VectorError ve = ComputeError(
           dataFrame.VectorColumnName( "Observations" ),
           dataFrame.VectorColumnName( "Predictions" ) );
       std::cout << "rho " << ve.rho << " RMSE " << ve.RMSE
                 << " MAE " << ve.MAE << std::endl << std::endl;</pre>
   }
    catch ( const std::exception & e ) {
      std::cout << "Exception caught in main:\n";</pre>
      std::cout << e.what() << std::endl;</pre>
      return -1;
   catch (...) {
      std::cout << "Unknown exception caught in main.\n";</pre>
      return -1;
   }
   std::cout << "Normal termination.\n";</pre>
   return 0;
}
```

Code Notes

- 1) The OSX XCode compiler/linker seems to be incompatible with the C++ standard implementation allowing template classes to be distributed into declarations (.h) and implementation (.cc). To support OSX, DataFrame.h contains both declarations and implementations. See: etc/libstdc++_Notes.txt.
- 2) The code relies heavily on class and data containers without explicit heap allocation. This facilitates garbage collection. If the code encounters massive data objects/large problems, this may warrant investigation.
- 3) SMap uses the LAPACK (http://www.netlib.org/lapack/explore-html/index.html) routine dgelss() to solve the local linear maps by singular value decomposition.

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.