

# cppEDM Version 1.0.1 November 28 2019

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.

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## Introduction

cppEDM is a C++ implementation of empirical dynamic modeling (EDM) algorithms. Core algorithms are listed in table 1. It is primarily a functional programming implementation with 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 shares many high-level design attributes with the devEDM Python package. cppEDM has Python and R interfaces with the pyEDM and rEDM packages.

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>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 correlation, MAE, RMSE	

## Installation

cppEDM is available at [github.com/SugiharaLab/cppEDM](https://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

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 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 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>	Create DataFrame from csv file
WriteData(path, file)	string outputFilePath string outputFileName		Write DataFrame to file
Elements()		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()		map<string, size_t>	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.
DataFrameFromColumnIndex ( columns )	vector<size_t> columns	DataFrame<double>	Get DataFrame subset from column indices
DataFrameFromColumnNames ( columns )	vector<string> columns	DataFrame<double>	Get DataFrame subset from column names
WriteRow(row, array)	size_t row std::valarray<T> array		Write valarray to row
WriteColumn(col, array)	size_t col valarray<T> array		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
<code>pathIn</code>	string	<code>"./"</code>	Input data file path
<code>dataFile</code>	string	<code>""</code>	Data file name
<code>pathOut</code>	string	<code>"./"</code>	Output file path
<code>predictFile</code>	string	<code>""</code>	Prediction output file
<code>lib</code>	string	<code>""</code>	library start : stop row indices
<code>pred</code>	string	<code>""</code>	prediction start : stop row indices
<code>E</code>	int	0	Data dimension
<code>Tp</code>	int	0	Prediction interval (rows)
<code>knn</code>	int	0	Number nearest neighbors
<code>tau</code>	int	1	Embedding delay (rows)
<code>theta</code>	float	0	SMap localisation
<code>exclusionRadius</code>	int	0	Prediction vector exclusion row radius
<code>columns</code>	string	<code>""</code>	Column names or indices for prediction
<code>target</code>	string	<code>""</code>	Target library column name or index
<code>embedded</code>	bool	false	Is data an embedding?
<code>const_pred</code>	bool	false	Include non-projected forecast data
<code>verbose</code>	bool	false	Echo messages
<code>smapFile</code>	string	<code>""</code>	SMap coefficient output file
<code>multiview</code>	int	0	Number of ensembles, 0 = sqrt(N)
<code>libSizes_str</code>	string	<code>""</code>	CCM library sizes
<code>sample</code>	int	0	CCM number of random samples
<code>random</code>	bool	true	CCM use random samples?
<code>replacement</code>	bool	false	CCM sample with replacement?
<code>seed</code>	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.

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

```
//-----
// Overload 1: Explicit data file path/name
//-----
DataFrame<double> Simplex( std::string pathIn      = "./data/",
                          std::string dataFile    = "",
                          std::string pathOut     = "./",
                          std::string predictFile = "",
                          std::string lib         = "",
                          std::string pred        = "",
                          int           E         = 0,
                          int           Tp        = 1,
                          int           knn        = 0,
                          int           tau        = 1,
                          int           exclusionRadius = 0,
                          std::string columns    = "",
                          std::string target     = "",
                          bool          embedded  = false,
                          bool          const_pred = false,
                          bool          verbose   = true );

//-----
// Overload 2: DataFrame reference provided
//-----
DataFrame<double> Simplex( DataFrame< double > &dataFrameIn,
                          std::string pathOut      = "./",
                          std::string predictFile   = "",
                          std::string lib           = "",
                          std::string pred          = "",
                          int           E           = 0,
                          int           Tp          = 1,
                          int           knn          = 0,
                          int           tau          = 1,
                          int           exclusionRadius = 0,
                          std::string columns       = "",
                          std::string target        = "",
                          bool          embedded     = false,
                          bool          const_pred   = false,
                          bool          verbose      = true );
```

## SMap

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

SMap( ) returns a SMapValues structure:

```
struct SMapValues {
    DataFrame< double > predictions;
    DataFrame< double > coefficients;
};
```

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.

```
//-----
// 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 pred        = "",
                 int          E           = 0,
                 int          Tp          = 1,
                 int          knn         = 0,
                 int          tau         = 1,
                 double       theta       = 0,
                 int          exclusionRadius = 0,
                 std::string columns     = "",
                 std::string target      = "",
                 std::string smapFile    = "",
                 std::string derivatives = "", // Not implemented
                 bool         embedded    = false,
                 bool         const_pred  = false,
                 bool         verbose     = true );
```



```

//-----
// Overload 2: DataFrame reference provided
//-----
SMapValues SMap( DataFrame< double > &dataFrameIn,
                std::string pathOut          = "./",
                std::string predictFile      = "",
                std::string lib              = "",
                std::string pred             = "",
                int          E                = 0,
                int          Tp              = 1,
                int          knn             = 0,
                int          tau             = 1,
                double       theta           = 0,
                int          exclusionRadius = 0,
                std::string columns          = "",
                std::string target           = "",
                std::string smapFile         = "",
                std::string derivatives      = "", // Not implemented
                bool         embedded        = false,
                bool         const_pred      = false,
                bool         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 `replacement` is `true`, observation are selected with replacement. 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.

```
//-----  
// Overload 1: Explicit data file path/name  
//-----  
DataFrame<double> CCM( std::string pathIn      = "./data/",  
                      std::string dataFile   = "",  
                      std::string pathOut    = "./",  
                      std::string predictFile = "",  
                      int      E             = 0,  
                      int      Tp           = 0,  
                      int      knn          = 0,  
                      int      tau          = 1,  
                      std::string columns    = "",  
                      std::string target     = "",  
                      std::string libSizes   = "",  
                      int      sample       = 0,  
                      bool      random       = true,  
                      bool      replacement  = false,  
                      unsigned   seed        = 0,      // seed=0: use RNG  
                      bool      verbose     = true );
```

```

//-----
// Overload 2: DataFrame reference provided
//-----
DataFrame<double> CCM( DataFrame< double > &dataFrameIn,
                      std::string pathOut      = "./",
                      std::string predictFile  = "",
                      int      E               = 0,
                      int      Tp              = 0,
                      int      knn             = 0,
                      int      tau             = 1,
                      std::string columns      = "",
                      std::string target       = "",
                      std::string libSizes     = "",
                      int      sample          = 0,
                      bool      random         = true,
                      bool      replacement    = false,
                      unsigned  seed           = 0,      // seed=0: use RNG
                      bool      verbose       = true );

```

## 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 > Combo_rho;
    DataFrame< double > Predictions;
    std::vector< std::string > Combo_rho_table;
};
```

The `Combo_rho` DataFrame has  $E+3$  columns. The first  $E$  columns are the the column indices in the input data 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.

`Combo_rho_table` is a list of strings that include the multiview embedding column names in addition to the column indices and prediction statistics.

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.

`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  $E+1$ .

```
//-----
// 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      E              = 0,
                           int      Tp             = 1,
                           int      knn            = 0,
                           int      tau            = 1,
                           std::string columns     = "",
                           std::string target      = "",
                           int      multiview      = 0,
                           int      exclusionRadius = 0,
                           bool      verbose       = false,
                           unsigned  nThreads      = 4 );

//-----
// Overload 2: DataFrame provided
//-----
MultiviewValues Multiview( DataFrame< double >,
                           std::string pathOut    = "./",
                           std::string predictFile = "",
                           std::string lib         = "",
                           std::string pred        = "",
                           int      E              = 0,
                           int      Tp             = 1,
                           int      knn            = 0,
                           int      tau            = 1,
                           std::string columns     = "",
                           std::string target      = "",
                           int      multiview      = 0,
                           int      exclusionRadius = 0,
                           bool      verbose       = false,
                           unsigned  nThreads      = 4 );
```

## 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      = "./data/",  
                                  std::string dataFile    = "",  
                                  std::string pathOut     = "./",  
                                  std::string predictFile = "",  
                                  std::string lib         = "",  
                                  std::string pred        = "",  
                                  int maxE               = 10,  
                                  int Tp                 = 1,  
                                  int tau                = 1,  
                                  std::string columns     = "",  
                                  std::string target      = "",  
                                  bool embedded          = false,  
                                  bool verbose           = true,  
                                  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        = "",  
                                  int maxE               = 10,  
                                  int Tp                 = 1,  
                                  int tau                = 1,  
                                  std::string columns     = "",  
                                  std::string target      = "",  
                                  bool embedded          = false,  
                                  bool verbose           = true,  
                                  unsigned 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      = "./data/",  
                                   std::string dataFile    = "",  
                                   std::string pathOut      = "./",  
                                   std::string predictFile  = "",  
                                   std::string lib          = "",  
                                   std::string pred        = "",  
                                   int maxTp               = 10,  
                                   int E                  = 0,  
                                   int tau                 = 1,  
                                   std::string columns     = "",  
                                   std::string target      = "",  
                                   bool embedded           = false,  
                                   bool verbose            = true,  
                                   unsigned nThreads       = 4 );  
  
//-----  
// Overload 2: DataFrame reference provided  
//-----  
DataFrame<double> PredictInterval( DataFrame< double > &dataFrameIn,  
                                   std::string pathOut      = "./",  
                                   std::string predictFile  = "",  
                                   std::string lib          = "",  
                                   std::string pred        = "",  
                                   int maxTp               = 10,  
                                   int E                  = 0,  
                                   int tau                 = 1,  
                                   std::string columns     = "",  
                                   std::string target      = "",  
                                   bool embedded           = false,  
                                   bool verbose            = true,  
                                   unsigned nThreads       = 4 );
```

## PredictNonlinear

Evaluate SMap prediction skill for localisation parameters  $\theta$  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".

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  
//-----  
DataFrame<double> PredictNonlinear( std::string pathIn      = "./data/",  
                                     std::string dataFile   = "",  
                                     std::string pathOut     = "./",  
                                     std::string predictFile = "",  
                                     std::string lib         = "",  
                                     std::string pred        = "",  
                                     std::string theta       = "",  
                                     int E                  = 0,  
                                     int Tp                 = 1,  
                                     int tau                 = 1,  
                                     std::string columns     = "",  
                                     std::string target      = "",  
                                     bool embedded          = false,  
                                     bool verbose           = true,  
                                     unsigned nThreads      = 4 );  
  
//-----  
// 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       = "",  
                                     int E                  = 0,  
                                     int Tp                 = 1,  
                                     int tau                 = 1,  
                                     std::string columns     = "",  
                                     std::string target      = "",  
                                     bool embedded          = false,  
                                     bool verbose           = true,  
                                     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:

```
struct VectorError {  
    double rho;  
    double RMSE;  
    double MAE;  
};  
  
//-----  
//-----  
VectorError ComputeError( std::valarray< double > obsIn,  
                           std::valarray< double > 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 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. 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.

## Example Application

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

```
// g++ TestApp.cc -o TestApp -std=c++11 -g -I../src -L../lib -lstdc++ -LEDM

#include "Common.h"

int main( int argc, char *argv[] ) {

    try {
        //-----
        // embedded=false : Simplex embeds data file columns to E=3
        //-----
        DataFrame<double> dataFrame =
            Simplex( "../data/",          // pathIn
                    "block_3sp.csv",      // dataFile
                    "./",                 // pathOut
                    "Block3sp_E3.csv",    // predictFile
                    "1 100",               // lib
                    "101 195",            // pred
                    3,                     // E
                    1,                     // Tp
                    0,                     // knn
                    1,                     // tau
                    0,                     // exclusionRadius
                    "x_t y_t z_t",        // columns
                    "x_t",                 // target
                    false,                 // embedded
                    false,                 // const_predict
                    true );                // verbose

        dataFrame.MaxRowPrint() = 12; // Set number of rows to print
        std::cout << dataFrame;

        VectorError ve = ComputeError(
            dataFrame.VectorColumnName( "Observations" ),
            dataFrame.VectorColumnName( "Predictions" ) );

        std::cout << "rho " << ve.rho << "  RMSE " << ve.RMSE
                    << "  MAE " << ve.MAE << std::endl << std::endl;

    }

    catch ( const std::exception& e ) {
        std::cout << "Exception caught in main:\n";
        std::cout << e.what() << std::endl;
        return -1;
    }
    catch (...) {
        std::cout << "Unknown exception caught in main.\n";
        return -1;
    }

    std::cout << "Normal termination.\n";

    return 0;
}
```

## Code Notes

- 1) The OSX XCode compiler/linker seems to be incompatible with the C++11 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. However, using copy-on-return for large data objects is likely a performance issue. 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

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