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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	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
EmbedDimension()	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 Eigen C++ template library (<a href="eigen.tuxfamily.org/">eigen.tuxfamily.org/</a>). 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></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
<pre>MaxRowPrint()</pre>		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
DataFrameFromColumnIndex ( columns )	vector <size_t></size_t>	DataFrame <double></double>	Get DataFrame subset from column indices
DataFrameFromColumnNames ( columns )	vector <string></string>	DataFrame <double></double>	Get DataFrame subset from column names
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	n n	Data file name
pathOut	string	"./"	Output file path
predictFile	string	n n	Prediction output file
lib	string	" "	library start : stop row indices
pred	string	n n	prediction start : stop row indices
E	int	0	Data dimension
Tp	int	0	Prediction interval (rows)
knn	int	0	Number nearest neighbors
tau	int	1	Embedding delay (rows)
theta	float	0	SMap localisation
exclusionRadius	int	0	Prediction vector exclusion row 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
multiview	int	0	Number of ensembles, $0 = sqrt(N)$
libSizes_str	string	II II	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?
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\*(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
                                tau = 0,
                   int
                                columns = "",
                  std::string
                                verbose = false );
                  bool
// Called from Embed to create the time-delay embedding
//----
DataFrame< double > MakeBlock ( DataFrame< double >
                                      dataFrame,
                     int
                                      Ε,
                                      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
                      std::string columns = ""
                     bool const_pred = false,
bool verbose = true )
                                            = 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 = "",
                     bool const_pred = false,
bool verbose = true )
                                            = 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.

1ib 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 csy 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
                              \mathbf{E}
                              Тp
                  int
                 int knn
int tau
double theta
int exclusion
                                               = 0,
                              exclusionRadius = 0,
                  std::string columns
                                               = ""
                                               = "",
                  std::string target
                  std::string target - ,
std::string smapFile = "",
                 std::string derivatives = "",
bool embedded = false,
bool const_pred = false,
bool verbose = true)
                                                       // Not implemented
                                               = true );
```

```
// Overload 2: DataFrame reference provided
//----
SMapValues SMap( DataFrame< double > &dataFrameIn,
           std::string lib
                               = "",
                              = "",
           std::string pred
           int
                   E
                              = 0,
                               = 1,
           int
                    Тр
           int
                   knn
                              = 0,
                              = 1,
           int
                   tau
           double theta = 0,
int exclusionRadius = 0,
= ""
           std::string columns = "",
                              = "",
           std::string target
                                     // Not implemented
                             = false,
                    const_pred
           bool
           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 radomly 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 2: DataFrame reference provided
//-----
DataFrame<double> CCM( DataFrame< double > &dataFrameIn,
                                     = "./",
                   std::string pathOut
                   std::string predictFile = "",
                                         = 0,
                             \mathbf{E}
                   int
                   int
                             qT
                                         = 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,
                                        = 0,
                                                // seed=0: use RNG
                   unsigned seed
                   bool
                                        = true );
                             verbose
```

#### 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 csy 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
                                         = "",
                           E
Tp
knn
                     int
                     int
                                         = 1,
                     int
                                         = 0,
                             tau
                     int
                     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
                                          = 0,
                     int
                          E
                            Тp
                     int
                     int
                             knn
                                          = 0,
                        tau
                     int
                     std::string columns
                                          = "",
                     std::string target
                         multiview = 0,
exclusionRadius = 0,
verbose = false,
                     int
                     int
                     bool
                     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
                               maxE
Tp
tau
                           int
                           int
                                    tau
                           int
                           std::string columns = "", std::string target = "",
                           bool embedded bool verbose
                                              = false,
                                              = 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
int Tp
int tau
                           std::string columns
std::string target
                                              = "",
                           bool embedded
bool verbose
unsigned nThreads
                                              = false,
                                              = true,
                                              = 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 = "",
                              std::string pred
                              int maxTp
                              int
                                       E
                              int
                                        tau
                              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
                                     maxTp
                                                   = 10,
                              int
                              int
                                         E
                              int
                                        tau
                              std::string columns = "",
std::string target = "",
                              bool embedded
bool verbose
unsigned nThreads
                                                   = false,
                                                   = true,
                                                   = 4);
```

#### **PredictNonlinear**

Evaluate SMap prediction skill for localisation parameters  $\theta$  specifed 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
                              E
                       int
                       int
                              Тp
                       int
                              tau
                       std::string columns = ""
                                     = "",
                       std::string target
                       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
                       int
                              Тp
                              tau
                       int
                       std::string columns
                       std::string target
                       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 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, adust 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
                                     // E
                    3,
                                     // Tp
                    1,
                                     // knn
                    Ο,
                                     // tau
                    1,
                                     // exclusionRadius
                   "x_t y_t z_t",
"x_t",
                                     // columns
                                     // target
                   false,
                                     // embedded
                   false,
                                     // const predict
                                     // verbose
                   true );
       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;
   }
   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++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) Eigen template library. The recommended SVD solver is the BDCSVD that scales to large problems. However, the Eigen documentation states:

This algorithm is unlikely to provide accurate results when compiled with unsafe math optimizations. For instance, this concerns Intel's compiler (ICC), which performs such optimization by default unless you compile with the -fp-model precise option. Likewise, the -ffast-math option of GCC or clang will significantly degrade accuracy.

See: <u>eigen.tuxfamily.org/dox/group</u> <u>TutorialLinearAlgebra</u>
Note that in gcc -ffast-math is not turned on by any -O option besides -Ofast. cppEDM uses -O3.

4) Eigen template library. Eigen allows replacement of it's internal template library routines with direct calls to BLAS/LAPACK libraries. See: https://eigen.tuxfamily.org/dox/TopicUsingBlasLapack.html This may offer performance and stability advantages. The Lapack SVD routine dgesdd\_() can also be called directly without the need for Eigen, see etc/lapack\_dgesdd.cc.

### References

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