

MatrixLibrary

1.0

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Chapter 1

MatrixLibrary

1.1 Introduction

MatrixLibrary is a matrix library with basic linear algebra functionality including eigenvalue decompositions for symmetric matrices.

1.2 Features

- [Matrix](#) arithmetic
- Householder tridiagonalization
- QL eigenvalue solver
- Symmetry Check
- Transpose
- HDF5 output

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

std::domain_error	
InvalidMatrixSize	10
InvalidMatrixSize	10
EigsymResult	9
Matrix	10
QLEigenResult	16
TridiagonalResult	17

Chapter 3

Class Index

3.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

EigsymResult	Final eigenvalues and eigenvectors of matrix	9
InvalidMatrixSize	Exception thrown this error if the matrix size is invalid for specified operation	10
Matrix	Matrix class with basic linear algebra operations	10
QLEigenResult	Result of QL Algorithm	16
TridiagonalResult	Result of Householder Tridiagonalization	17

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

include/custom_exception.hpp	19
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include/matrix.h	21
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src/benchmark.hpp	23
src/custom_exception.hpp	19
src/helper_func.cpp	24
src/matrix_basic_func.cpp	25
src/matrix_eigendecomp.cpp	25
src/matrix_operators.cpp	26
src/matrix_utilfuncs.cpp	26

Chapter 5

Class Documentation

5.1 EigsymResult Struct Reference

Final eigenvalues and eigenvectors of matrix.

```
#include <matrix.h>
```

Collaboration diagram for EigsymResult:

Public Attributes

- [vec eigenvalues](#)
- [Matrix eigenvectors](#)

5.1.1 Detailed Description

Final eigenvalues and eigenvectors of matrix.

This code is adapted from Numerical Recipes

5.1.2 Member Data Documentation

5.1.2.1 eigenvalues

```
vec EigsymResult::eigenvalues
```

5.1.2.2 eigenvectors

```
Matrix EigsymResult::eigenvectors
```

The documentation for this struct was generated from the following file:

- include/[matrix.h](#)

5.2 InvalidMatrixSize Class Reference

Exception thrown this error if the matrix size is invalid for specified operation.

```
#include <custom_exception.hpp>
```

Inheritance diagram for InvalidMatrixSize:

Collaboration diagram for InvalidMatrixSize:

Public Member Functions

- [InvalidMatrixSize](#) (const std::string &what_arg)
- [InvalidMatrixSize](#) (const std::string &what_arg)

5.2.1 Detailed Description

Exception thrown this error if the matrix size is invalid for specified operation.

5.2.2 Constructor & Destructor Documentation

5.2.2.1 InvalidMatrixSize() [1/2]

```
InvalidMatrixSize::InvalidMatrixSize (
    const std::string & what_arg ) [inline]
```

5.2.2.2 InvalidMatrixSize() [2/2]

```
InvalidMatrixSize::InvalidMatrixSize (
    const std::string & what_arg ) [inline]
```

The documentation for this class was generated from the following files:

- include/[custom_exception.hpp](#)
- src/[custom_exception.hpp](#)

5.3 Matrix Class Reference

[Matrix](#) class with basic linear algebra operations.

```
#include <matrix.h>
```


Public Member Functions

- [Matrix](#) (int rows, int cols)
*Construct a matrix of size (row * cols)*
- [Matrix](#) ()
- [Matrix](#) (const [vec](#) &values, int rows, int cols)
*Construct a matrix of size (row * cols) with data.*
- [Matrix](#) ([vec](#) &&values, int rows, int cols)
- int [get_num_rows](#) () const
- int [get_num_cols](#) () const
- int [get_size](#) () const
- const [vec](#) & [get_data](#) () const
- double & [operator](#)() (int x, int y)
Access a matrix element at (row, col)
- const double & [operator](#)() (int x, int y) const
Const reference to the matrix element at (row, col)
- bool [operator==](#) (const [Matrix](#) &other) const
- [Matrix](#) [operator+](#) (const [Matrix](#) &other) const
- [Matrix](#) [operator-](#) (const [Matrix](#) &other) const
- [Matrix](#) [operator*](#) (const [Matrix](#) &other) const
- [Matrix](#) [operator*](#) (double s) const
- bool [is_symmetric](#) (double tol) const
- [Matrix](#) [transpose](#) () const
- [TridiagonalResult](#) [householder_tridiagonalize](#) (bool yesvecs=true) const
- [QLEigenResult](#) [QL](#) ([vec](#) d, [vec](#) e) const
- [EigsymResult](#) [eigsym](#) () const

Static Public Member Functions

- static [Matrix](#) [Ones](#) (int rows, int cols)
Fill matrix of specified size with 1's.
- static [Matrix](#) [Zeros](#) (int rows, int cols)
Fill matrix of specified size with 0's.
- static [Matrix](#) [Random](#) (int rows, int cols)
Fill matrix of specific size with random doubles from [0.0, 1.0)
- static [Matrix](#) [Identity](#) (int n)
*Create square identity matrix with dimensions n*n.*
- static [Matrix](#) [diagmat](#) (const [vec](#) &vector)
- static [Matrix](#) [diagmat](#) (const [Matrix](#) &mat)
- static void [save_hdf5](#) (const [Matrix](#) &data, const std::string &filename, const std::string &dataset_name)
- static void [save_hdf5](#) (const [vec](#) &data, const std::string &filename, const std::string &dataset_name)

Private Attributes

- int [num_rows](#)
- int [num_cols](#)
- int [size](#)
- [vec](#) [matrix](#)

5.3.1 Detailed Description

[Matrix](#) class with basic linear algebra operations.

The matrix class stores elements in contiguous memory to improve cache locality. This class supports multiplication, addition, subtraction, symmetry checks, transposing matrix, saving to HDF5 file and eigenvalue decompositions for symmetric matrices.

5.3.2 Constructor & Destructor Documentation

5.3.2.1 `Matrix()` [1/4]

```
Matrix::Matrix (
    int rows,
    int cols )
```

Construct a matrix of size (row * cols)

5.3.2.2 `Matrix()` [2/4]

```
Matrix::Matrix ( )
```

5.3.2.3 `Matrix()` [3/4]

```
Matrix::Matrix (
    const vec & values,
    int rows,
    int cols )
```

Construct a matrix of size (row * cols) with data.

5.3.2.4 `Matrix()` [4/4]

```
Matrix::Matrix (
    vec && values,
    int rows,
    int cols )
```

5.3.3 Member Function Documentation

5.3.3.1 `diagmat()` [1/2]

```
Matrix Matrix::diagmat (
    const Matrix & mat ) [static]
```

5.3.3.2 diagmat() [2/2]

```
Matrix Matrix::diagmat (
    const vec & vector ) [static]
```

5.3.3.3 eigsym()

```
EigsymResult Matrix::eigsym ( ) const
```

5.3.3.4 get_data()

```
const vec & Matrix::get_data ( ) const
```

5.3.3.5 get_num_cols()

```
int Matrix::get_num_cols ( ) const
```

5.3.3.6 get_num_rows()

```
int Matrix::get_num_rows ( ) const
```

5.3.3.7 get_size()

```
int Matrix::get_size ( ) const
```

5.3.3.8 householder_tridiagonalize()

```
TridiagonalResult Matrix::householder_tridiagonalize (
    bool yesvecs = true ) const
```

5.3.3.9 Identity()

```
Matrix Matrix::Identity (
    int n ) [static]
```

Create square identity matrix with dimensions $n \times n$.

5.3.3.10 is_symmetric()

```
bool Matrix::is_symmetric (
    double tol = 1e-12 ) const
```

5.3.3.11 Ones()

```
Matrix Matrix::Ones (
    int rows,
    int cols ) [static]
```

Fill matrix of specified size with 1's.

5.3.3.12 operator() [1/2]

```
double & Matrix::operator() (
    int x,
    int y )
```

Access a matrix element at (row, col)

Parameters

<i>x</i>	row index (0-based)
<i>y</i>	column index (0-based)

Returns

reference to the matrix element

Exceptions

<i>OutOfBounds</i>	exception if the indices are invalid
--------------------	--------------------------------------

5.3.3.13 operator() [2/2]

```
const double & Matrix::operator() (
    int x,
    int y ) const
```

Const reference to the matrix element at (row, col)

5.3.3.14 operator*() [1/2]

```
Matrix Matrix::operator* (
    const Matrix & other ) const
```

5.3.3.15 operator*() [2/2]

```
Matrix Matrix::operator* (
    double s ) const
```

5.3.3.16 operator+()

```
Matrix Matrix::operator+ (
    const Matrix & other ) const
```

5.3.3.17 operator-()

```
Matrix Matrix::operator- (
    const Matrix & other ) const
```

5.3.3.18 operator==()

```
bool Matrix::operator== (
    const Matrix & other ) const
```

5.3.3.19 QL()

```
QLEigenResult Matrix::QL (
    vec d,
    vec e ) const
```

5.3.3.20 Random()

```
Matrix Matrix::Random (
    int rows,
    int cols ) [static]
```

Fill matrix of specific size with random doubles from [0.0, 1.0)

5.3.3.21 save_hdf5() [1/2]

```
void Matrix::save_hdf5 (
    const Matrix & data,
    const std::string & filename,
    const std::string & dataset_name ) [static]
```

5.3.3.22 save_hdf5() [2/2]

```
void Matrix::save_hdf5 (
    const vec & data,
    const std::string & filename,
    const std::string & dataset_name ) [static]
```

5.3.3.23 transpose()

```
Matrix Matrix::transpose ( ) const
```

5.3.3.24 Zeros()

```
Matrix Matrix::Zeros (
    int rows,
    int cols ) [static]
```

Fill matrix of specified size with 0's.

5.3.4 Member Data Documentation

5.3.4.1 matrix

```
vec Matrix::matrix [private]
```

5.3.4.2 num_cols

```
int Matrix::num_cols [private]
```

5.3.4.3 num_rows

```
int Matrix::num_rows [private]
```

5.3.4.4 size

```
int Matrix::size [private]
```

The documentation for this class was generated from the following files:

- [include/matrix.h](#)
- [src/matrix_basic_func.cpp](#)
- [src/matrix_eigendecomp.cpp](#)
- [src/matrix_operators.cpp](#)
- [src/matrix_utilfuncs.cpp](#)

5.4 QLEigenResult Struct Reference

Result of QL Algorithm.

```
#include <matrix.h>
```

Collaboration diagram for QLEigenResult:

Public Attributes

- [vec eigenvalues](#)
- [Matrix Q_ql](#)

5.4.1 Detailed Description

Result of QL Algorithm.

This code is adapted from Numerical Recipes

5.4.2 Member Data Documentation

5.4.2.1 eigenvalues

`vec` QLEigenResult::eigenvalues

5.4.2.2 Q_ql

`Matrix` QLEigenResult::Q_ql

The documentation for this struct was generated from the following file:

- include/[matrix.h](#)

5.5 TridiagonalResult Struct Reference

Result of Householder Tridiagonalization.

```
#include <matrix.h>
```

Collaboration diagram for TridiagonalResult:

Public Attributes

- `vec` d
- `vec` e
- `Matrix` Q_house

5.5.1 Detailed Description

Result of Householder Tridiagonalization.

This code is adapted from Numerical Recipes

5.5.2 Member Data Documentation

5.5.2.1 d

`vec` TridiagonalResult::d

5.5.2.2 e

`vec` TridiagonalResult::e

5.5.2.3 Q_house

`Matrix` TridiagonalResult::Q_house

The documentation for this struct was generated from the following file:

- include/[matrix.h](#)

Chapter 6

File Documentation

6.1 include/custom_exception.hpp File Reference

#include <stdexcept>

Include dependency graph for custom_exception.hpp: This graph shows which files directly or indirectly include this file:

Classes

- class [InvalidMatrixSize](#)

Exception thrown this error if the matrix size is invalid for specified operation.

6.2 custom_exception.hpp

[Go to the documentation of this file.](#)

```
00001 #pragma once
00002 #include <stdexcept>
00003
00008 class InvalidMatrixSize : public std::domain_error {
00009 public:
00010     InvalidMatrixSize(const std::string& what_arg) : std::domain_error(what_arg)
00011     {}
00012 };
```

6.3 src/custom_exception.hpp File Reference

#include <stdexcept>

Include dependency graph for custom_exception.hpp:

Classes

- class [InvalidMatrixSize](#)

Exception thrown this error if the matrix size is invalid for specified operation.

6.4 custom_exception.hpp

[Go to the documentation of this file.](#)

```
00001 #pragma once
00002 #include <stdexcept>
00003
00004 class InvalidMatrixSize : public std::domain_error {
00005 public:
00006     InvalidMatrixSize(const std::string& what_arg) : std::domain_error(what_arg)
00007     {}
00008 };
```

6.5 include/helper_func.hpp File Reference

This graph shows which files directly or indirectly include this file:

Functions

- double [SIGN](#) (double a, double b)
*Return a value equivalent to $|a| * \text{sign}(b)$*
- double [pythag](#) (double a, double b)
Computes $\text{sqrt}(a^2 + b^2)$ without destructive overflow or underflow.

6.5.1 Function Documentation

6.5.1.1 pythag()

```
double pythag (
    double a,
    double b )
```

Computes $\text{sqrt}(a^2 + b^2)$ without destructive overflow or underflow.

Helper function for eigenvalue and eigenvector calculation. Adapted from Numerical Recipes.

6.5.1.2 SIGN()

```
double SIGN (
    double a,
    double b )
```

Return a value equivalent to $|a| * \text{sign}(b)$

Helper function for eigenvalue and eigenvector calculation. Adapted from Numerical Recipes.

6.6 helper_func.hpp

[Go to the documentation of this file.](#)

```
00001 #pragma once
00002
00009 double SIGN(double a, double b);
00010
00017 double pythag(double a, double b);
```

6.7 include/matrix.h File Reference

```
#include <iostream>
#include <vector>
#include <limits>
#include "custom_exception.hpp"
#include "helper_func.hpp"
#include <cmath>
#include <iomanip>
#include <stdexcept>
#include <random>
```

Include dependency graph for matrix.h: This graph shows which files directly or indirectly include this file:

Classes

- class [Matrix](#)
Matrix class with basic linear algebra operations.
- struct [TridiagonalResult](#)
Result of Householder Tridiagonalization.
- struct [QLEigenResult](#)
Result of QL Algorithm.
- struct [EigsymResult](#)
Final eigenvalues and eigenvectors of matrix.

Typedefs

- typedef std::vector< double > [vec](#)
Alias for vector of doubles, used for matrix storage.

Functions

- std::ostream & [operator<<](#) (std::ostream &out, const [Matrix](#) &M)

6.7.1 Typedef Documentation

6.7.1.1 vec

```
typedef std::vector<double> vec
```

Alias for vector of doubles, used for matrix storage.

6.7.2 Function Documentation

6.7.2.1 operator<<()

```
std::ostream & operator<< (
    std::ostream & out,
    const Matrix & M )
```

6.8 matrix.h

[Go to the documentation of this file.](#)

```

00001 #pragma once
00002
00003 #include <iostream>
00004 #include <vector>
00005 #include <limits>
00006 #include "custom_exception.hpp"
00007 #include "helper_func.hpp" // numerical recipes helper functions
00008 #include <cmath>
00009 #include <iomanip>
00010 #include <stdexcept>
00011 #include <random>
00012
00033 typedef std::vector<double> vec;
00034
00035 // Forward declarations of global result types
00036 struct TridiagonalResult;
00037 struct EigsymResult;
00038 struct QLEigenResult;
00039
00049 class Matrix {
00050 private:
00051     int num_rows;
00052     int num_cols;
00053     int size;
00054     vec matrix;
00055
00056 public:
00057     // === Constructors ===
00061     Matrix(int rows, int cols);
00062     Matrix();
00066     Matrix(const vec& values, int rows, int cols);
00067     Matrix(vec&& values, int rows, int cols);
00068
00069     // === Factory Methods ===
00073     static Matrix Ones(int rows, int cols);
00074
00078     static Matrix Zeros(int rows, int cols);
00079
00083     static Matrix Random(int rows, int cols);
00084
00088     static Matrix Identity(int n);
00089
00090     // === Accessors ===
00091     int get_num_rows() const;
00092     int get_num_cols() const;
00093     int get_size() const;
00094     const vec& get_data() const;
00095
00096     // === Operators ===
00106     double& operator()(int x, int y);
00107
00111     const double& operator()(int x, int y) const;
00112
00113     bool operator==(const Matrix& other) const;
00114     Matrix operator+(const Matrix& other) const;
00115     Matrix operator-(const Matrix& other) const;
00116     Matrix operator*(const Matrix& other) const;
00117     Matrix operator*(double s) const;
00118
00119     // === Linear Algebra Functionality ===
00120     static Matrix diagmat(const vec& vector);
00121     static Matrix diagmat(const Matrix& mat);
00122     bool is_symmetric(double tol) const;
00123     Matrix transpose() const;
00124     TridiagonalResult householder_tridiagonalize(bool yesvecs = true) const;
00125     QLEigenResult QL(vec d, vec e) const;
00126     EigsymResult eigsym() const;
00127
00128     // === Saving to HDF5 File ===
00129     static void save_hdf5(const Matrix& data, const std::string& filename, const std::string&
dataset_name);
00130     static void save_hdf5(const vec& data, const std::string& filename, const std::string&
dataset_name);
00131
00132 };
00133
00139 struct TridiagonalResult {
00140     vec d; // diagonal elements
00141     vec e; // off-diagonal elements
00142     Matrix Q_house; // orthogonal transformation matrix
00143 };
00144

```

```

00150 struct QLEigenResult {
00151     vec eigenvalues;
00152     Matrix Q_ql;
00153 };
00154
00160 struct EigsymResult {
00161     vec eigenvalues;
00162     Matrix eigenvectors;
00163 };
00164
00165 // === Printing Functionality ===
00166 std::ostream& operator<<(std::ostream& out, const Matrix & M);

```

6.9 include/print_vec.hpp File Reference

```

#include <iostream>
#include <vector>
#include <iomanip>

```

Include dependency graph for print_vec.hpp:

Functions

- `std::ostream & operator<< (std::ostream &out, const std::vector< double > &v)`
Overload print operator for vector.

6.9.1 Function Documentation

6.9.1.1 operator<<()

```

std::ostream & operator<< (
    std::ostream & out,
    const std::vector< double > & v ) [inline]

```

Overload print operator for vector.

6.10 print_vec.hpp

[Go to the documentation of this file.](#)

```

00001 #pragma once
00002 #include <iostream>
00003 #include <vector>
00004 #include <iomanip>
00005
00009 inline std::ostream& operator<<(std::ostream& out, const std::vector<double>& v) {
00010     out << std::fixed << std::setprecision(4);
00011     for (double x : v) {
00012         out << x << "\n";
00013     }
00014     return out;
00015 }

```

6.11 src/benchmark.hpp File Reference

```

#include <vector>
#include <chrono>

```

Include dependency graph for benchmark.hpp:

6.12 benchmark.hpp

[Go to the documentation of this file.](#)

```
00001 #pragma once
00002
00003 #include <vector>
00004 #include <chrono>
00005
00006 template <typename T>
00007 long benchmark_time(T func, int iterations=25) {
00008     std::vector<double> vec_diff;
00009     vec_diff.reserve(iterations);
00010     for (int i = 0; i < iterations; ++i) {
00011         auto start = std::chrono::steady_clock::now();
00012         func();
00013         auto end = std::chrono::steady_clock::now();
00014
00015         // Convert to nanoseconds
00016         double diff = std::chrono::duration<double, std::nano>(end - start).count();
00017         vec_diff.push_back(diff);
00018     }
00019
00020     // get average
00021     double avg = 0.0;
00022     for (double val : vec_diff) {
00023         avg += val;
00024     }
00025     // return time diff in microseconds
00026     return avg / vec_diff.size();
00027 }
00028
00029 // need to implement L2 norm for this benchmarking
00030 template <typename T>
00031 long benchmark_acc(T func1, T func2) {
00032     auto diff = func1() - func2();
00033     return diff;
00034 }
```

6.13 src/helper_func.cpp File Reference

```
#include "helper_func.hpp"
#include <cmath>
```

Include dependency graph for helper_func.cpp: This graph shows which files directly or indirectly include this file:

Functions

- double [SIGN](#) (double a, double b)
*Return a value equivalent to $|a| * \text{sign}(b)$*
- double [pythag](#) (const double a, const double b)
Computes $\text{sqrt}(a^2 + b^2)$ without destructive overflow or underflow.

6.13.1 Function Documentation

6.13.1.1 pythag()

```
double pythag (
    double a,
    double b )
```

Computes $\text{sqrt}(a^2 + b^2)$ without destructive overflow or underflow.

Helper function for eigenvalue and eigenvector calculation. Adapted from Numerical Recipes.

6.13.1.2 SIGN()

```
double SIGN (
    double a,
    double b )
```

Return a value equivalent to $|a| * \text{sign}(b)$

Helper function for eigenvalue and eigenvector calculation. Adapted from Numerical Recipes.

6.14 helper_func.cpp

[Go to the documentation of this file.](#)

```
00001 #include "helper_func.hpp"
00002 #include <cmath>
00003
00004 double SIGN(double a, double b) {
00005     if ( b >= 0.0 ) {
00006         return std::fabs(a);
00007     } else {
00008         return -std::fabs(a);
00009     }
00010 }
00011
00012 double pythag(const double a, const double b) {
00013     // computes sqrt(a^2 + b^2) without destructive underflow or overflow
00014     double absa = std::abs(a);
00015     double absb = std::abs(b);
00016     if (absa > absb) {
00017         return absa * sqrt(1.0 + (absb/absa)*(absb/absa));
00018     } else {
00019         return absb * sqrt(1.0 + (absa/absb)*(absa/absb));
00020     }
00021 }
```

6.15 src/matrix_basic_func.cpp File Reference

```
#include "matrix.h"
#include <algorithm>
Include dependency graph for matrix_basic_func.cpp:
```

6.16 src/matrix_eigendecomp.cpp File Reference

```
#include "matrix.h"
#include "helper_func.cpp"
#include <cmath>
#include <stdexcept>
#include <limits>
#include <algorithm>
#include <numeric>
Include dependency graph for matrix_eigendecomp.cpp:
```

6.17 src/matrix_operators.cpp File Reference

```
#include "matrix.h"
#include <algorithm>
#include <iomanip>
#include <cmath>
#include <limits>
Include dependency graph for matrix_operators.cpp:
```

Functions

- `std::ostream & operator<< (std::ostream &out, const Matrix &M)`

6.17.1 Function Documentation

6.17.1.1 `operator<<()`

```
std::ostream & operator<< (
    std::ostream & out,
    const Matrix & M )
```

6.18 src/matrix_utilfuncs.cpp File Reference

```
#include "matrix.h"
#include <cmath>
#include <highfive/H5File.hpp>
Include dependency graph for matrix_utilfuncs.cpp:
```


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