# Free Implementation of GMRES in C++

Version 0.2

Fri Jul 7 2023

Kelly Black <kjblack@gmail.com>

# **Contents**

1	Over	view												1
	1.1	Introdu	ction			 	 	 	 	 		 		1
	1.2	Calling	the GMR	ES Subroutine		 	 	 	 	 		 		1
	1.3	The Op	peration C	ass		 	 	 	 	 		 		2
	1.4	The Ap	proximation	on Class		 	 	 	 	 		 		3
	1.5	The Pr	econdition	er Class		 	 	 	 	 		 		4
2	GMR	ES												5
3	Class	s Index												7
						 	 	 	 	 		 		7
4	File I	ndev												9
•			t			 	 	 	 	 		 		9
		=				 			 	 				·
5			mentation											11
				ber > Class Te										11
		5.1.1		Description .										11
		5.1.2												12
		5.1.3		PTION										12
		5.1.4		tor & Destructo										12
			5.1.4.1	ArrayUtils() .										12
		5.1.5		Function Docu										12
			5.1.5.1	delfivetensor	•									12
			5.1.5.2	delfourtensor	**									12
			5.1.5.3	delonetensor	•									13
			5.1.5.4	delthreetenso	**									13
			5.1.5.5	deltwotensor	•									13
			5.1.5.6	fivetensor()										13
			5.1.5.7	fourtensor()										14
			5.1.5.8	onetensor().										14
			5.1.5.9	threetensor()										14
			5.1.5.10	twotensor() .		 	 ٠.	 	 	 	•	 	 ٠	15
6	File [	Docume	entation											17
	6.1	<b>GMRE</b>	S.h File R	eference		 	 	 	 	 		 		17
		6.1.1	Detailed	Description .		 	 	 	 	 		 		17
		6.1.2	LICENSE			 	 	 	 	 		 		17
		6.1.3	DESCRI	PTION		 	 	 	 	 		 		18
		6.1.4	Function	Documentation	١	 	 	 	 	 		 		18
			6.1.4.1	GMRES()		 	 	 	 	 		 		18
			6.1.4.2	Update()										18
	6.2	GMRE	S.h			 	 	 	 	 		 		19
	6.3			nce										21
		6.3.1		Description .										21
	6.4	util.h .												21

<u>iv</u>	CONTENTS
Bibliography	23
Index	25

# **Overview**

#### 1.1 Introduction

The codes given here are a free implementation of the Generalized Minimal Residual Method (GMRES) in c++. The method is fully described by Saad[5] and Kelley[4]. The code given here is based on the pseudo code given by Barrett *et al*[1]. The codes were adapted to c++ after examining the matlab codes by Burkardt[2]. This specific implementation makes use of restarts, and it was most influenced by the code available from the United States' National Institute of Standards and Technology[3].

The GMRES algorithm is defined in the file GMRES.h. The algorithm is given in a template function, named GMRES. The subroutine assumes that three classes are defined that include several specific operators and functions. There is an additional subroutine called by GMRES named Update. This subroutine is used to generate an updated approximation based on the Krylov subspace generated within the GMRES subroutine.

There is an additional set of subroutines that are used within the GMRES subroutine. These routines are defined in the files util.h and util.cpp. The file util.h includes the file util.cpp. Both files are assumed to be in the same directory as the GMRES.h file.

In this overview the call for the GMRES routine is first given, and then the three required classes are stated in turn. First the Operation class is discussed, then the Approximation class, and finally the Preconditioner class is discussed. Each class must implement specific operations and define a given set of methods. The expectations are given within each section.

# 1.2 Calling the GMRES Subroutine

The GMRES routine is named GMRES, and the definition for the method is given in Listing 1.1. There are seven parameters for the function. The first four parameters are pointers to the respective classes. The next three parameters dictate the behaviour and limits of the GMRES implementation and include the number of vectors in the Krylov subspace, the number of restarts, and the tolerance respectively.

Listing 1.1: The definition for the GMRES routine.

```
template < class Operation , class Approximation , class Preconditioner , class Double > int GMRES (Operation * linearization , //! < Performs the linearization of the PDE on the approximation . Approximation * solution , //! < The approximation to the linear system. (and initial estimate!) Approximation * rhs , //! < the right hand side of the equation to solve . Preconditioner * precond , //! < The preconditioner used for the linear system . int krylovDimension , //! < The number of vectors to generate in the Krylov subspace . int numberRestarts , //! < Number of times to repeat the GMRES iterations . Double tolerance //! < How small the residual should be to terminate the GMRES iterations .
```

The basic idea is that an approximation to a linear system is to be generated. The system can be represented by

$$L\vec{x} = \vec{b}. \tag{1.1}$$

2 Overview

The parameters in the subroutine correspond to the following symbols in equation (1.1):

 $egin{array}{lll} L &=& ext{linearization}, \ & ec{x} &=& ext{solution}, \ & ec{b} &=& ext{rhs}. \end{array}$ 

The parameter in the Operation class, linearization, is used to implement the action of the matrix multiplied by a vector. The vector is given by an object in the Approximation class which includes the initial estimate, solution, and the right hand side, rhs. The variable solution is updated, and it is changed by calling the routine.

The final class, Preconditioner, is used to implement a preconditioner for the system. The assumption is that the preconditioned system is in the form

$$P^{-1}L\vec{x} = P^{-1}\vec{b}.$$

The GMRES algorithm requires that the operator, precond in the GMRES routine, be used to generate a sequence of vectors given by

$$\vec{v}_{n+1} = L\hat{v}_n,$$

where  $\hat{v}_n$  is a normalized vector that is orthogonal to the previous vectors generated. The GMRES subroutine calculates this under the assumption that the system to solve is given by the system

$$P\vec{v}_{n+1} = L\hat{v}_n, \tag{1.2}$$

where the routine solves for the vector  $\vec{v}_{n+1}$ .

Listing 1.2: The definition for the Update routine.

Finally, the file includes an additional subroutine, <code>Update</code>. This subroutine is used to perform the back-solve and update to determine the next approximation to the linear system. This is used within the <code>GMRES</code> subroutine and is not expected to be called by another routine.

# 1.3 The Operation Class

The first class examined is the Operation class. This class is used to perform the actions equivalent to a matrix multiply. It is assumed that this is in the form of a right multiply, i.e.

 $L \cdot \vec{x}$ .

Listing 1.3: An example of the multiply operation defined for the Operation class.

The Operation class must have a number of operations defined. In particular the class should have the multiply operator defined. An example of the required definition is given in Listing 1.3.

Methods	Operations
norm	+
getN	_
2 constructors	+=
ахру	=
	*

Table 1.1: The methods and operations that must be defined for the Approximation class.

# 1.4 The Approximation Class

The Approximation class is used to keep track of the approximation to the solution to the linear system. It is the class used to store  $\vec{x}$  as well as  $\vec{b}$  in equation (1.1). It is assumed that the Approximation class has a number of methods and operations defined, and the complete list is given in Table 1.1.

Examples of the basic form for the definitions are given in Listing 1.4. Note the types of the arguments. For example, the addition operator is for the sum of two objects from the Approximation class while the multiplication operator is for an object from the Approximation class multiplied on the right by a real valued variable.

Listing 1.4: An example of the operations that must be defined for the Approximation class.

There are four methods that must be defined for the Approximation class. Examples of the definitions are shown in Listing 1.5. Note that there are two constructors that must be called. The first is a constructor that requires the number of entries to allocate in the approximation. The second is a constructor that makes a copy of the Approximation object passed to it.

Also note that the axpy method is a method that adds a scalar multiplied by another Approximation object to the current object. This method is used in the modified Gramm-Schmidt orthogonalization of the vectors that make up the Krylov subspace.

Listing 1.5: An example of the methods that must be defined for the Approximation class.

```
Approximation::Approximation(int size)
{
...
}
Approximation::Approximation(const Approximation& oldCopy)
{
```

4 Overview

```
double Approximation::norm(const Approximation& v1)
         double norm = v1.getEntry(0)*v1.getEntry(0);
         int lupe;
         for (lupe=v1.getN(); lupe>0; --lupe)
                           norm += v1.getEntry(lupe)*v1.getEntry(lupe);
         return(sqrt(norm));
}
int Approximation::getN() const
  return(N);
void Approximation::axpy(Approximation* vector,
                                             double multiplier)
{
         int lupe:
         for (lupe=getN(); lupe>=0;--lupe)
                           setEntry\,(\,getEntry\,(\,lupe\,) + multiplier\,\star\,vector\,-\!\!>\!getEntry\,(\,lupe\,)\;, lupe\,)\,;
                  }
```

# 1.5 The Preconditioner Class

The final class is the Preconditioner class. This class only requires one method, the solve method. This method is used to solve the system given in equation (1.2). An example of the definition is given in Listing 1.6. Notice that it returns an object from the Approximation class.

Listing 1.6: An example of the solve method that must be defined for the Preconditioner class.

```
Approximation Preconditioner::solve(const Approximation &current)
        Approximation multiplied (current);
         // Perform the forward solve to invert the first part of the
         // Cholesky decomposition.
         intermediate[0] = current.getEntry(0)/vector[0][0];
         for (lupe=1; lupe <= getN(); + + lupe)
                 intermediate[lupe] =
                          (current.getEntry(lupe)-vector[lupe][1]*intermediate[lupe-1])
                           /vector[lupe][0];
         // Perform the backwards solve for the Cholesky decomposition.
         multiplied \, (getN \, ()) \, = \, intermediate \, [getN \, ()] / \, vector \, [getN \, ()] [0] \, ;
         for (lupe=getN()-1; lupe>=0; --lupe) \\ multiplied(lupe) = (intermediate[lupe]-multiplied(lupe+1)*vector[lupe+1][1]) 
                          /vector[lupe][0];
         \ensuremath{//} The previous solves wiped out the boundary conditions. Restore
         // the left and right boundaru condition before sending the result
         // back.
         multiplied(0) = current.getEntry(0);
        multiplied (getN()) = current.getEntry(getN());
         return (multiplied);
```

# **GMRES**

A c++ implementation of the GMRES method for approximating the solution to a linear system.

This set of software is composed of Several include files that define template functions to implement the GMRES method. The code is based on the GMRES method with restarts. The code is influenced by the IML++ implementation as well as John Burkardt's MATLAB implementation.

Please see the file latex/refman.pdf for more details on how to use the code. An example of how to use the code can be found in the example directory.

This software is licensed under a BSD license and is free for anyone to use and/or adapt.

6 GMRES

# **Class Index**

3.1	Class	ı	ist
<b>J.</b> I	Olass	_	. 1 3 (

Here are the classes, structs, unions and interfaces with brief descriptions:	
ArrayUtils< number >	
Header file for the basic utilities associated with managing arrays	1

8 Class Index

# File Index

14	C:Ia		L
4. I	CIIC	List	ı

Here is a list of all documented files with brief descriptions:	
GMRES.h	
Template files for implementing a GMRES algorithm to solve a linear sytem	17
util.h	21

10 File Index

# **Class Documentation**

# 5.1 ArrayUtils < number > Class Template Reference

Header file for the basic utilities associated with managing arrays. #include < util.h>

#### **Public Member Functions**

• ArrayUtils ()

#### Static Public Member Functions

- static number \*\*\*\* fivetensor (int n1, int n2, int n3, int n4, int n5)
- static number \*\*\*\* fourtensor (int n1, int n2, int n3, int n4)
- static number \*\*\* threetensor (int n1, int n2, int n3)
- static number \*\* twotensor (int n1, int n2)
- static number \* onetensor (int n1)
- static void delfivetensor (number \*\*\*\*\*u)
- static void delfourtensor (number \*\*\*\*u)
- static void delthreetensor (number \*\*\*u)
- static void deltwotensor (number \*\*u)
- static void delonetensor (number \*u)

## 5.1.1 Detailed Description

```
template<class number> class ArrayUtils< number>
```

Header file for the basic utilities associated with managing arrays.

Author

```
Kelly Black kjblack@gmail.com
```

Version

0.1

Copyright

BSD 2-Clause License

12 Class Documentation

#### 5.1.2 LICENSE

Copyright (c) 2014, Kelly Black All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- 2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT HOLDER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

#### 5.1.3 DESCRIPTION

Class to provide a set of basic utilities that are used by numerous other classes.

This is the definition (header) file for the ArrayUtils class. It includes the definitions for the methods that are used to construct and delete arrays used in a variety of other classes.

#### 5.1.4 Constructor & Destructor Documentation

#### 5.1.4.1 ArrayUtils()

```
template<class number >
ArrayUtils< number >::ArrayUtils ( ) [inline]
Base constructor for the ArrayUtils class.
```

There is not anything to do so this is an empty method.

#### 5.1.5 Member Function Documentation

# 5.1.5.1 delfivetensor()

```
template<class number >
void ArrayUtils< number >::delfivetensor (
```

number \*\*\*\*\* u ) [static] Template for deleting a five dimensional array.

#### **Parameters**

u pointer to the array to be deleted.

# 5.1.5.2 delfourtensor()

```
template<class number >
void ArrayUtils< number >::delfourtensor (
```

number \*\*\*\* u ) [static]
Template for deleting a four dimensional array.

#### **Parameters**

pointer to the array to be deleted.

## 5.1.5.3 delonetensor()

```
template<class number >
void ArrayUtils< number >::delonetensor (
                          [static
```

number \* u ) [static]
Template for deleting a one dimensional array.

#### **Parameters**

u pointer to the array to be deleted.

# 5.1.5.4 delthreetensor()

```
{\tt template}{<}{\tt class\ number}\,>\,
void ArrayUtils< number >::delthreetensor (
```

number \*\*\* u ) [static]
Template for deleting a three dimensional array.

#### **Parameters**

pointer to the array to be deleted.

## 5.1.5.5 deltwotensor()

```
{\tt template}{<}{\tt class\ number}\,>\,
void ArrayUtils< number >::deltwotensor (
```

<u>number \*\* u ) [static]</u>
Template for deleting a two dimensional array.

#### **Parameters**

pointer to the array to be deleted.

## 5.1.5.6 fivetensor()

```
template<class number >
\verb|number| ***** ArrayUtils < \verb|number| >:: fivetensor (
               int n1,
               int n2,
               int n3,
               int n4,
```

int n5) [static]
Template for allocating a five dimensional array.

#### **Parameters**

n1	Number of entries for the first dimension.
n2	Number of entries for the second dimension.
n3	Number of entries for the third dimension.
n4	Number of entries for the fourth dimension.
n5	Number of entries for the fifth dimension.

14 **Class Documentation** 

#### Returns

A pointer to the array created.

## 5.1.5.7 fourtensor()

```
template<class number >
number **** ArrayUtils< number >::fourtensor (
             int n1,
             int n2,
             int n3,
```

 $\frac{\text{int } n4 \text{ ) } [\text{static}]}{\text{Template for allocating a four dimensional array.}}$ 

#### **Parameters**

n	1	Number of entries for the first dimension.
n.	2	Number of entries for the second dimension.
n	3	Number of entries for the third dimension.
n-	4	Number of entries for the fourth dimension.

#### Returns

A pointer to the array created.

# 5.1.5.8 onetensor()

```
{\tt template}{<}{\tt class\ number}\,>\,
number * ArrayUtils< number >::onetensor (
```

int n1 ) [static]
Template for allocating a one dimensional array.

## **Parameters**

Number of entries for the dimension.

#### Returns

A pointer to the array.

## 5.1.5.9 threetensor()

```
{\tt template}{<}{\tt class\ number}\,>\,
number *** ArrayUtils< number >::threetensor (
                      int n1,
                      int n2,
\frac{\text{int } n3 \text{ }) \text{ } [\text{static}]}{\text{Template for allocating a three dimensional array.}}
```

## **Parameters**

n1	Number of entries for the first dimension.
n2	Number of entries for the second dimension.
n3	Number of entries for the third dimensions.

## Returns

A pointer to the array created.

## 5.1.5.10 twotensor()

 $\frac{\text{int } n2 \text{ ) } [\text{static}]}{\text{Template for allocating a two dimensional array.}}$ 

## **Parameters**

n1	Number of entries for the first dimension.
n2	Number of entries for the second dimension.

# Returns

A pointer to the array created.

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

- util.h
- util.cpp

16 Class Documentation

# **File Documentation**

# 6.1 GMRES.h File Reference

Template files for implementing a GMRES algorithm to solve a linear sytem.

```
#include "util.h"
#include <cmath>
#include <vector>
```

#### **Functions**

- template < class Approximation , class Double >
   void Update (Double \*\*H, Approximation \*x, Double \*s, std::vector < Approximation > \*v, int dimension)
- template < class Operation, class Approximation, class Preconditioner, class Double >
   int GMRES (Operation \*linearization, Approximation \*solution, Approximation \*rhs, Preconditioner \*precond,
   int krylovDimension, int numberRestarts, Double tolerance)

## 6.1.1 Detailed Description

Template files for implementing a GMRES algorithm to solve a linear sytem.

**Author** 

```
Kelly Black kjblack@gmail.com
```

Version

0.2

Copyright

BSD 2-Clause License

## 6.1.2 LICENSE

Copyright (c) 2014, Kelly Black All rights reserved.

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

- Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
- 2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.

18 File Documentation

THIS SOFTWARE IS PROVIDED BY THE COPYRIGHT HOLDERS AND CONTRIBUTORS "AS IS" AND ANY EXPRESS OR IMPLIED WARRANTIES, INCLUDING, BUT NOT LIMITED TO, THE IMPLIED WARRANTIES OF MERCHANTABILITY AND FITNESS FOR A PARTICULAR PURPOSE ARE DISCLAIMED. IN NO EVENT SHALL THE COPYRIGHT HOLDER OR CONTRIBUTORS BE LIABLE FOR ANY DIRECT, INDIRECT, INCIDENTAL, SPECIAL, EXEMPLARY, OR CONSEQUENTIAL DAMAGES (INCLUDING, BUT NOT LIMITED TO, PROCUREMENT OF SUBSTITUTE GOODS OR SERVICES; LOSS OF USE, DATA, OR PROFITS; OR BUSINESS INTERRUPTION) HOWEVER CAUSED AND ON ANY THEORY OF LIABILITY, WHETHER IN CONTRACT, STRICT LIABILITY, OR TORT (INCLUDING NEGLIGENCE OR OTHERWISE) ARISING IN ANY WAY OUT OF THE USE OF THIS SOFTWARE, EVEN IF ADVISED OF THE POSSIBILITY OF SUCH DAMAGE.

#### 6.1.3 DESCRIPTION

This file includes the template functions necessary to implement a restarted GMRES algorithm. This is based on the pseudo code given in the book Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition [1].

Also, some changes were implemented based on the matlab code by John Burkardt [2] http://people.sc.fsu.edu/~jbur The idea for using a template came from the IML++ code [3] http://math.nist.gov/iml++/ Also, the method for calculating the entries for the Givens rotation matrices came from the IML++ code as well.

Additional sources that informed this work are Tim Kelley's book Iterative Methods for Linear and Nonlinear Equations [4] Another book is is Yousef Saad's book Iterative Methods for Sparse Linear Systems [5]

#### 6.1.4 Function Documentation

#### 6.1.4.1 GMRES()

Implementation of the restarted GMRES algorithm. Follows the algorithm given in the book Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition.

#### Returns

The number of iterations required. Returns zero if it did not converge.

#### **Parameters**

linearization	Performs the linearization of the PDE on the approximation.
solution	The approximation to the linear system. (and initial estimate!)
rhs	the right hand side of the equation to solve.
precond	The preconditioner used for the linear system.
krylovDimension	The number of vectors to generate in the Krylov subspace.
numberRestarts	Number of times to repeat the GMRES iterations.
tolerance	How small the residual should be to terminate the GMRES iterations.

# 6.1.4.2 Update()

template<class Approximation , class Double >

6.2 GMRES.h 19

Update the current approximation to the solution to the linear system. This assumes that the update is created using a GMRES routine, and the upper Hessenberg matrix has been transformed to an upper diagonal matrix already. Note that it changes the values of the values in the coefficients vector, s, which means that the s vector cannot be reused after this without being re-initialized.

# 6.2 GMRES.h

Go to the documentation of this file.

```
00001
00067 #include "util.h"
00068 #include <cmath>
00069 #include <vector>
00070
00080 template <class Approximation, class Double >
00081 void Update
00082 (Double **H.
                          //<! The upper diagonal matrix constructed in the GMRES routine.
                         //<! The current approximation to the linear system.
00083
      Approximation *x,
                          //<! The vector e_1 that has been multiplied by the Givens rotations.
00084
00085
      00086 int dimension)
                        //<! The number of vectors in the basis for the Krylov subspace.
00087 {
00088
00089
       // Solve for the coefficients, i.e. solve for c in
00090
       // H*c=s, but we do it in place.
00091
       int lupe;
00092
       for (lupe = dimension; lupe >= 0; --lupe)
00093
               s[lupe] = s[lupe]/H[lupe][lupe];
00094
00095
               for (int innerLupe = lupe - 1; innerLupe >= 0; --innerLupe)
00096
00097
                       // Subtract off the parts from the upper diagonal of the
00098
00099
                       s[innerLupe] -= s[lupe]*H[innerLupe][lupe];
00100
                   }
00101
           }
00102
00103
       // Finally update the approximation.
00104
         typename std::vector<Approximation>::iterator ptr = v->begin();
       00105
00106
00107 }
00108
00109
00110
00118 template<class Operation, class Approximation, class Preconditioner, class Double>
00119 int GMRES
00120 (Operation* linearization,
00121 Approximation* solution, 00122 Approximation* rhs,
      Approximation* rhs,
      Preconditioner* precond,
00124 int krylovDimension,
00125
      int numberRestarts,
00126 Double tolerance
00127
00128 {
00129
00130
         // Allocate the space for the givens rotations, and the upper
00131
          // Hessenburg matrix.
                         = ArrayUtils<Double>::twotensor(krylovDimension+1,krylovDimension);
00132
         Double **H
00133
00134
            The Givens rotations include the sine and cosine term. The
00135
         // cosine term is in column zero, and the sine term is in column
00136
00137
         Double **givens = ArrayUtils<Double>::twotensor(krylovDimension+1,2);
00138
00139
         // The vector s the right hand side for the system that the matrix
00140
         // H satisfies in order to minimize the residual over the Krylov
00141
          // subspace.
00142
         Double *s = ArrayUtils<Double>::onetensor(krylovDimension+1);
00143
00144
         // Determine the residual and allocate the space for the Krylov
00145
         // subspace.
00146
         std::vector<Approximation> V(krylovDimension+1,
00147
                                     Approximation(solution->getN()));
```

20 File Documentation

```
Approximation residual = precond->solve((*rhs)-(*linearization)*(*solution));
                                   = residual.norm();
00149
00150
          Double normRHS
                                   = rhs->norm();
00151
00152
           // variable for keeping track of how many restarts had to be used.
00153
          int totalRestarts = 0:
00154
00155
          if(normRHS < 1.0E-5)
00156
              normRHS = 1.0;
00157
00158
          // Go through the requisite number of restarts.
00159
          int iteration = 1:
00160
          while( (--numberRestarts >= 0) && (rho > tolerance*normRHS))
00161
00162
00163
                   // The first vector in the Krylov subspace is the normalized
00164
                   // residual.
                   V[0] = residual * (1.0/rho);
00165
00166
00167
                   // Need to zero out the s vector in case of restarts
00168
                   // initialize the s vector used to estimate the residual.
00169
                   for(int lupe=0;lupe<=krylovDimension;++lupe)</pre>
00170
                       s[lupe] = 0.0;
00171
                   s[0] = rho;
00172
00173
                   // Go through and generate the pre-determined number of vectors
00174
                   // for the Krylov subspace.
00175
                   for( iteration=0; iteration<krylovDimension; ++iteration)</pre>
00176
00177
                            // Get the next entry in the vectors that form the basis for
00178
                            // the Krylov subspace.
00179
                            V[iteration+1] = precond->solve((*linearization)*V[iteration]);
00180
00181
                            // Perform the modified Gram-Schmidt method to orthogonalize
00182
                            // the new vector.
00183
                            int row;
00184
                            typename std::vector<Approximation>::iterator ptr = V.begin();
00185
                            for (row=0; row<=iteration; ++row)</pre>
00186
00187
                                    H[row][iteration] = Approximation::dot(V[iteration+1], *ptr);
00188
                                     //subtract H[row][iteration]*V[row] from the current vector
                                    V[iteration+1].axpy(&(*ptr++),-H[row][iteration]);
00189
00190
00191
00192
                            H[iteration+1][iteration] = V[iteration+1].norm();
00193
                            V[iteration+1] *= (1.0/H[iteration+1][iteration]);
00194
                           // Apply the Givens Rotations to insure that H is // an upper diagonal matrix. First apply previous \,
00195
00196
00197
                            // rotations to the current matrix.
00198
                           double tmp;
00199
                            for (row = 0; row < iteration; row++)</pre>
00200
00201
                                    tmp = givens[row][0]*H[row][iteration] +
00202
                                    00203
00204
00205
                                    H[row][iteration] = tmp;
00206
00207
                            \ensuremath{//} Figure out the next Givens rotation.
00208
00209
                            if(H[iteration+1][iteration] == 0.0)
00210
00211
                                     // It is already lower diagonal. Just leave it be....
00212
                                    givens[iteration][0] = 1.0;
00213
                                    givens[iteration][1] = 0.0;
00214
00215
                            else if (fabs(H[iteration+1][iteration]) > fabs(H[iteration][iteration]))
00216
00217
                                    // The off diagonal entry has a larger
00218
                                    // magnitude. Use the ratio of the
00219
                                    // diagonal entry over the off diagonal.
                                    tmp = H[iteration][iteration]/H[iteration+1][iteration];
00220
                                    givens[iteration][1] = 1.0/sqrt(1.0+tmp*tmp);
givens[iteration][0] = tmp*givens[iteration][1];
00221
00222
00223
00224
                            else
00225
00226
                                    // The off diagonal entry has a smaller
00227
                                    // magnitude. Use the ratio of the off
                                    // diagonal entry to the diagonal entry.
00228
                                    tmp = H[iteration+1][iteration]/H[iteration][iteration];
00229
                                    givens[iteration][0] = 1.0/sqrt(1.0+tmp*tmp);
givens[iteration][1] = tmp*givens[iteration][0];
00230
00231
00232
00233
00234
                            // Apply the new Givens rotation on the
```

6.3 util.h File Reference 21

```
// new entry in the uppper Hessenberg matrix.
00236
                              tmp = givens[iteration][0]*H[iteration][iteration] +
00237
                                  givens[iteration][1]*H[iteration+1][iteration];
                             H[iteration+1][iteration] = -givens[iteration][1]*H[iteration][iteration] +
    givens[iteration][0]*H[iteration+1][iteration];
00238
00239
00240
                             H[iteration][iteration] = tmp;
00241
00242
                              // Finally apply the new Givens rotation on the s
00243
                              \begin{array}{l} tmp = givens[iteration][0] *s[iteration] + givens[iteration][1] *s[iteration+1]; \\ s[iteration+1] = -givens[iteration][1] *s[iteration] + \\ \end{array} 
00244
00245
      givens[iteration][1]*s[iteration+1];
00246
                             s[iteration] = tmp;
00247
00248
                             rho = fabs(s[iteration+1]);
00249
                             if(rho < tolerance*normRHS)</pre>
00250
00251
                                       // We are close enough! Update the approximation.
                                       Update(H, solution, s, &V, iteration);
00252
00253
                                       ArrayUtils<double>::deltwotensor(givens);
00254
                                       ArrayUtils<double>::deltwotensor(H);
00255
                                       ArrayUtils<double>::delonetensor(s);
                                       //delete [] V;
//tolerance = rho/normRHS;
00256
00257
00258
                                       return(iteration+totalRestarts*krylovDimension);
00259
00260
00261
                         } // for(iteration)
00262
                    \ensuremath{//} We have exceeded the number of iterations. Update the
00263
00264
                    // approximation and start over.
00265
                    totalRestarts += 1;
00266
                    Update(H, solution, s, &V, iteration-1);
00267
                    residual = precond->solve((*linearization)*(*solution) - (*rhs));
00268
                    rho = residual.norm();
00269
00270
                } // while(numberRestarts,rho)
00271
00272
00273
           ArrayUtils<double>::deltwotensor(givens);
00274
           ArrayUtils<double>::deltwotensor(H);
00275
           ArrayUtils<double>::delonetensor(s);
00276
           //delete [] V;
00277
           //tolerance = rho/normRHS;
00278
00279
           if(rho < tolerance*normRHS)</pre>
00280
               return(iteration+totalRestarts*krylovDimension);
00281
00282
           return(0);
00283 }
00284
```

# 6.3 util.h File Reference

#include "util.cpp"

# Classes

class ArrayUtils < number >

Header file for the basic utilities associated with managing arrays.

## 6.3.1 Detailed Description

# 6.4 util.h

# Go to the documentation of this file.

```
00001 #ifndef UTILROUTINE
00002 #define UTILROUTINE
00003
00004
00055 template <class number>
00056 class ArrayUtils
00057 {
00058
00059 public:
00060
00067 ArrayUtils(){};
```

22 File Documentation

```
00068
00069
                 \ensuremath{//} Define the methods used to allocate the memory for and define
                 // beline the methods used to allocate the memory for and define // multi-dimensional arrays.

static number *****fivetensor(int n1,int n2,int n3,int n4,int n5);

static number ****fourtensor(int n1,int n2,int n3,int n4);

static number ***threetensor(int n1,int n2,int n3);

static number **twotensor(int n1,int n2);
00070
00071
00072
00073
00074
00075
                 static number *onetensor(int n1);
00076
                 // Define the methods used to delete the memory that was allocated // for multi-dimensional arrays. static void delfivetensor(number ******u);
00077
00078
00079
                 static void delfourtensor(number ****u);
static void delthreetensor(number ****u);
08000
00081
00082
                 static void deltwotensor(number **u);
00083
                 static void delonetensor(number *u);
00084
00085 };
00086
00087
00088 #include "util.cpp"
00089
00090
00091 #endif
00092
```

# **Bibliography**

- [1] R. Barrett, M. Berry, T. F. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, R. Pozo, C. Romine, and H. Van der Vorst. *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods, 2nd Edition.* SIAM, Philadelphia, PA, 1994. 1, 18
- [2] John Burkardt. gmres\_r.m, November 2014. based on a code by Tim Kelley found at http://people.sc.fsu.edu/~jburkardt/m\_src/toms866/solvers/gmres\_r.m. 1, 18
- [3] IML++. Gmres.h, November 2014. found at http://math.nist.gov/iml++/. 1, 18
- [4] Tim Kelley. Iterative Methods for Linear and Nonlinear Equations. SIAM, Philadelphia, PA, 2004. 1, 18
- [5] Yousef Saad. *Iterative Methods for Sparse Linear Systems*. SIAM, Philadelphia, PA, second edition, 2003. 1, 18

24 BIBLIOGRAPHY

# Index

```
ArrayUtils
    ArrayUtils< number >, 12
ArrayUtils< number >, 11
    ArrayUtils, 12
    delfivetensor, 12
    delfourtensor, 12
    delonetensor, 13
    delthreetensor, 13
    deltwotensor, 13
    fivetensor, 13
    fourtensor, 14
    onetensor, 14
    threetensor, 14
    twotensor, 15
delfivetensor
    ArrayUtils< number >, 12
delfourtensor
    ArrayUtils< number >, 12
delonetensor
    ArrayUtils< number >, 13
delthreetensor
    ArrayUtils< number >, 13
deltwotensor
    ArrayUtils< number >, 13
fivetensor
    ArrayUtils< number >, 13
fourtensor
    ArrayUtils< number >, 14
GMRES
    GMRES.h, 18
GMRES.h, 17
    GMRES, 18
    Update, 18
onetensor
    ArrayUtils< number >, 14
threetensor
    ArrayUtils< number >, 14
twotensor
    ArrayUtils< number >, 15
Update
    GMRES.h, 18
util.h, 21
```