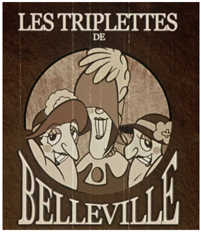
CS319: Scientific Computing (with C++)

Niall Madden (Niall.Madden@NUIGalway.ie)

Week 10: Sparse Matrices, and The STL

9am, 20 April, and 4pm, 21 April, 2021



CS319 – Week 10: Sparse Matrices, and The STL

Start of ...

PART 0: Assessment for CS319

Part 0: Assessment for CS319

I have tweaked the original assessment plan for CS319:

1. 50% based on lab assignments:
   - 10% for each of Lab 2 and Lab 3;
   - 15% for each of Lab 4+5 and Lab 7.
2. 50% based on your project work.

IS THAT OK?

Projects: Your project will consist of

1. An idea you select/propose, in (1:1) discussion with me;
2. A demonstration of various programming techniques in C++, including, minimally, coding your own class(es);
3. You will submit an initial, 250 word project proposal by Friday. (Word count is indicative: I won't check).
4. You will submit a 3 page project report along with your code. (DEADLINE???)
5. The report should be organised as follows.
   - 5.1 A summary of what you have done. This should be 300-500 words, and written in a non-technical style: anyone should be able to understand it. The emphasis should be on the problem solved, and why it is interesting, and not on the code.
   - 5.2 A technical discussion of the code.
   - 5.3 A note on what you have learned/discovered.
   - 5.4 An example of typical input and output.
   - 5.5 Details any limitations of your code that you have noted, and a comparison with your original project proposal.
   - 5.6 The highlights of your code: What took the most effort? What are you most proud of?

   The report must be in PDF and submitted here (via TurnItIn)

The code for your project is a chance for your to show your skills in C++ programming, and in scientific computing.
Each project will be independently negotiated with Niall.
Each will involve, at the very least, all of the following

1. An external data source, so that you can show your expertise in read from and/or writing to files.
2. A `class` (or set of classes) that you design yourself
3. An algorithm that preforms some type of useful calculation

The projects will be graded, and will contribute 50% to the over-all grade for CS319. The break-down of marks is as follows.

(a) Negotiating the project topic with Niall completed by 17:00, Friday 23 April [**5 Marks**]

(b) The project proposal completed by 17:00, Monday 26 April [**5 Marks**]

(c) C++ code [**25 Marks**]

(d) The Project report [**15 Marks**]

Some ideas for projects

Here is a random selection of topics. Their purpose is to stimulate discussion.

1. A class for storing *symmetric* matrices, and an implementation of the *Conjugate Gradients* algorithm for solving linear systems.
2. *LU*-decomposition for linear systems.
3. Problems in Cryptography I: Shift encryption, and decyphering it with a frequency analysis.
4. Other cryptography methods?
5. Algorithms on Graphs: minimum spanning trees, computing the chromatic number, searching (depth-first V breath-first), shortest path on weighted graphs, ...
6. Prime factorization with arbitrary precision integers.
7. Image enhancement: edge detection.
8. Data analysis - clustering methods
9. Triangulation of points in $\mathbb{R}^2$ (Delaunay).
10. ???

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END OF PART 0

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Start of ...

PART 1: Sparse Matrices

Part 1: Sparse Matrices

In Week 9 we looked at a social network analysis algorithm, PageRank For the problem to be interesting, our network should have thousands, perhaps millions, of nodes/vertices.

Compared to the over-all number of entries in the matrix, the **number of non-zeros** (**NNZs**) is relatively small. So it does not make sense to store them all. Instead, one uses one of the following formats:

- **Triplet** (which we'll look at presently),
- **Compressed Row Storage** (CRS) (after triplet)
- **Compressed Column Storage** (CCS)

And the following formats for very specialised matrices, which we won't study in CS319:

- **Block Compressed Row/Column Storage**
- **Compressed Diagonal Storage**
- **Skyline**

Although the representation and manipulation of sparse matrices is an major topic in Scientific Computing, there isn't a universally agreed definition of an (abstract) *sparse matrix*.

This is because, when coding, we should ask the question: **"When is it worth the effort to store a matrix in a sparse format, rather than in standard (dense) format?"**

The answer is often context-dependent. But roughly, use a sparse formal when

- The memory required by the sparse format is less then the "dense" (or "full") one;
- The expense of updating the sparse format is not excessive;
- Computing a `MatVec` is faster for a sparse matrix.

The basic idea for triplet form is: to store a **sparse** matrix with `NNZ` non-zeros we ...

- define `integer` arrays `I[NNZ]` and `J[NNZ]`,
- a `double` array `X[NNZ]`.
- Then entry a_{ij} is stored as `I[k]=i`, `J[k]=j`, `X[k]=`a_{ij}, for some k.

Example: write down the triplet form of the following matrix:

$$\begin{pmatrix} 1 & 0 & 11 & 0 \\ 1 & 0 & 2 & 0 \\ 9 & 19 & 0 & 29 \\ 0 & 0 & 0 & 5 \end{pmatrix}$$

Our next goal is implement a triplet matrix as a `class`. The main tasks are:

- Decide what private data elements are needed.
- Decide what public methods are needed.
- Implement a matrix-vector multiplication algorithm.

Discussion...

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END OF PART 1

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Start of ...

PART 2: **Coding** `triplet`

Part 2: Coding triplet

Triplet.h

```
// Triplet.h:  For 2021-CS319 Week 10
// Author: Niall Madden

#ifndef _TRIPLET_H_INCLUDED
#define _TRIPLET_H_INCLUDED

#include "Vector09.h"
#include "Matrix10.h"
```

Part 2: Coding `triplet`

Triplet.h

```
class Triplet {
  friend Triplet full2Triplet(Matrix &F, unsigned int NNZ_MAX);
private:
  unsigned int *I, *J;
  double *X;
  unsigned int N;
  unsigned int NNZ;
  unsigned int NNZ_MAX;

public:
  Triplet (unsigned int N, unsigned int nnz_max); // Constructor
  Triplet (const Triplet &t); // Copy constructor
  ~Triplet(void);

  Triplet &operator=(const Triplet &B); // overload assignment operator
```

Part 2: Coding triplet

Triplet.h

```
  unsigned int size(void) {return (N);};
  int where(unsigned int i, unsigned int j); // negative return on error
  unsigned int nnz(void) {return (NNZ);};
  unsigned int nnz_max(void) {return (NNZ_MAX);};

  double getij (unsigned int i, unsigned int j);
  void setij (unsigned int i, unsigned int j, double x);

  unsigned int getI (unsigned int k) { return I[k];};
  unsigned int getJ (unsigned int k) { return J[k];};
  double getX (unsigned int k) { return X[k];};

  Vector operator*(Vector u);
  void print(void);
};
#endif
```

Part 2: Coding triplet

Triplet.cpp

```
// Triplet.cpp  for 2021-CS319 Week 10
//   What: Methods for the Triplet class
// Author: Niall Madden
#include <iostream>
#include <iomanip>
#include "Vector09.h"
#include "Matrix10.h"
#include "Triplet.h"
```

Part 2: Coding triplet

Triplet.cpp (Constructor)

```
// Standard  constructor.
Triplet::Triplet (unsigned int N, unsigned int nnz_max) {
  this->N = N;
  this->NNZ_MAX = nnz_max;
  this->NNZ = 0;

  X = new double [nnz_max];
  I = new unsigned int [nnz_max];
  J = new unsigned int [nnz_max];
  for (unsigned int k=0; k<nnz_max; k++)  {
    I[k]=-1;
    J[k]=-1;
    X[k]=(double)NULL;
  }
}
```

Part 2: Coding triplet

When using a Triplet object to represent a matrix, T, we often need to find where in the array X, the value of $t_{i,j}$ is stored. That is done by the following function.

Triplet.cpp (where)

```
int Triplet::where(unsigned int i, unsigned int j)
{
  unsigned int k=0;
  do {
    if ( (I[k]==i) && (J[k]==j) )
      return(k);
    k++;
  } while (k<NNZ);
  return(-1);
}
```

Part 2: Coding triplet

Triplet.cpp (setij)

```
void Triplet::setij (unsigned int i, unsigned int j, double x)
{
  if (i>N-1)
    std::cerr << "Triplet::setij(): i Index out of bounds." << std::endl;
  else if (j>N-1)
    std::cerr << "Triplet::setij(): j Index out of bounds." << std::endl;
  else if (NNZ > NNZ_MAX-1)
    std::cerr << "Triplet::setij(): Matrix full." << std::endl;
  else
  {
    int k=where(i,j);
    if (k == -1)
    {
      I[NNZ]=i;
      J[NNZ]=j;
      X[NNZ]=x;
      NNZ++;
    }
    else
      X[k]=x;
  }
}
```

Part 2: Coding triplet

Triplet.cpp (operator *)

```
Vector Triplet::operator*(Vector u)
{
  Vector v(N); // v = A*u, where A is the implicitly passed Triplet
  v.zero();
  if (N != u.size())
    std::cerr << "Error: Triplet::operator* - dimension mismatch"
              << std::endl;
  else
    for (unsigned int k=0; k<NNZ; k++)
      v.seti(I[k], v.geti(I[k]) + X[k]*u.geti(J[k]));
  return(v);
}
```

. . . .

To demonstrate the use of the Triplet class, I've included a program called 01triplet_example which shows how to use the Jacobi method to solve a linear system where the matrix is stored in triplet format.

Part 2: Coding `triplet`

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END OF PART 2

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Start of ...

PART 3: CSS

The Compressed Column Sparse Format

Part 3: CCS

If we know that the entries in our matrix are stored in order, then it is possible to store the matrix more efficiently that in Triplet format. One way of doing this is to use **CCS**: **Compressed Column Storage**, also known as *Harwell-Boeing*

The matrix is stored in 3 vectors:

- a `double` array, x of length `nnz` ("number of nonzero entries") storing the non-zero entries matrix, in column-wise order.
- an `int` array, r of length `nnz` storing **row** index of the entries. That is, $x[k]$ would be found in row $r[k]$ of the full matrix.
- an `int` array, c of length $N + 1$, where $c[k]$ stores that starting point of column k as it appears in the arrays x and r, and $c[N] = nnz$.

Part 3: CCS

Example

Show how the matrix below would be stored in CCS

$$\begin{pmatrix} 2 & -1 & 0 & -2 \\ -3 & 5 & -1 & 0 \\ 0 & -2 & 4 & 0 \\ -3 & 0 & 0 & 4 \end{pmatrix}$$

Part 3: CCS

Matrix-vector multiplication

The process of multiplying a matrix (in CCS) by a vector is rather simple:

```
int index=0;
for (int col=0; col<N; col++)
   for (j=c[col]; j<c[col+1]; j++)
   {
     i=r[index];
     v[i] += x[index]*b[j];
     index++;
   }
```

. . . .

I don't provide code for implementing a CCS class here: that is an exercise.

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END OF PART 3

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Start of ...

PART 4: The Standard Template Library (STL)

Or “How not to reinventing the wheel

Part 4: The Standard Template Library   Not reinventing the wheel

During the semester, we've focused on designing classes that can be used to solve problems. These included classes: `Stack`, `Vector` and `Matrix`.

However, most of you worked out that, to some extent, these are already supported in C++. The motivations for reinventing them included

- our implementation is simple to use;
- we learned important aspects of C++/OOP;
- we needed to achieve specific tasks efficiently: this is particularly true of our design of sparse matrix classes.

Now we'll look at how to use the built-in implementation that comes with the C++ **Standard Template Library (STL)**.

The STL

The **STL** provides

(1) **Containers:** ways of collecting/storing items of some type (template....)

(2) **Iterators:** for accessing items in the containers

(3) **Algorithms:** for operating on the contents of containers, such as finding a particular item, or sorting (a subset) of them.

(4) **functors:** essentially, a class which defines the operator(). We won't say more than this right now.

We'll now look at examples of (1)–(3), and then consider an application to our Password Frequency Problem from a few weeks ago.

It has to be noted, though: the STL is not that easy to use. In particular the error messages generated are rather verbose and unhelpful.

Part 4: The Standard Template Library

A **container** stores objects/elements. These elements can have basic data-type (e.g., `char`, `int`, `double`, ...) or can be objects (e.g., `string`, or user-defined objects).

The most important types of containers are:

`vector`: an indexed sequence (often called "*random access*", though this would be better called "*arbitrary access*". All the items are of the same type. It can be resized, and have new items added to the end. One can also add items to positions not the end, but this is slow.

`set`: a collection of unique items (of the same type), stored in order. When defined relative to a user-defined class, an overloaded `operator<` (less than) must be provided for correct operation.

`multiset`: an ordered collection, like a set, but can have repeated values.

`list`: a doubly linked list.

`stack`:	a stack.
...	etc...

We'll focus on `set`s, `multiset`s and `vector`s.

An `iterator` is an object used to select (or move between) elements in a container.

We can think of them as pointers, that allow us to reference particular elements.

They come in particular flavours:

- forward, reverse, and bidirectional iterators;
- random-access/indexed-access iterators;
- input and output iterators;

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END OF PART 4

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Start of ...

PART 5: sets and multisets

Part 5: sets and multisets

To use a set or multiset, we must

```
#include <set>
```

Suppose we want to create a multiset to store strings (which just happen to be passwords...), and an iterator for it, we could define

```
std::multiset <std::string> multi_pwd;
std::multiset <std::string>::iterator multi_pwd_i;
```

To add an item to the (multi)set, we could used

```
multi_pwd.insert(MyString);
```

This will add the new string to the multiset, automatically choosing its position so that it remains ordered. (If we use a set, it gets inserted into the correct position, providing this does not result in duplication).

Part 5: `sets` and `multisets`

Other important methods include

- `begin()` (returns an iterator that points to the first element)
- `end()` (returns an iterator that points to *one past* the end of the set).
- `clear()` (remove contents)
- `count()` (count number of occuences)
- `empty()` (is the set empty?)
- `erase()` (remove an element, or range of elements)
- `find()` (locate an element; return an iterator)
- `size()` (number of elements)
- `swap()` (swap contents of two sets of same type)
- `for_each()` (apply a particular function to each item in a container)

Part 5: sets and multisets

An example of using begin and end with a set and multiset:

01set_and_multiset.cpp

```
int main(void )
{
  std::set <int> set_int;
  std::set <int>::iterator set_int_i;
  std::multiset <int> multi_int;
  std::multiset <int>::iterator multi_int_i;

  for (int i=0; i<=20; i+=3) // (0,3,6,9,12,15,18)
  {
    set_int.insert(i);
    multi_int.insert(i);
  }
  for (int i=20; i>0; i-=2) // (20,18,16,...,4,2)
  {
    set_int.insert(i);
    multi_int.insert(i);
  }
```

Part 5: sets and multisets

First, we will see how to iterate over the multiset:

01set_and_multiset.cpp

```
  std::cout << "The multiset has " << multi_int.size() <<
    " items." << std::endl;
  std::cout << "\t They are: ";
  for (multi_int_i = multi_int.begin();
       multi_int_i != multi_int.end();
       multi_int_i++)
    std::cout << std::setw(3) << *multi_int_i;
  std::cout << std::endl;
  std::cout << "\t 6 occurs " << multi_int.count(6) <<
    " time(s)." << std::endl;
```

The output is

```
The multiset has 17 items.
   They are:   0  2  3  4  6  6  8  9 10 12 12 14 15 16 18 18 20
   6 occurs 2 times.
```

Part 5: sets and multisets

Next we will iterate over the set:

02set_and_multiset.cpp

```cpp
std::cout << "The set has " << set_int.size() <<
  " items." << std::endl;
std::cout << "\t They are: ";
for (set_int_i = set_int.begin();
     set_int_i != set_int.end();
     set_int_i++)
  std::cout << std::setw(3) << *set_int_i;
std::cout << std::endl << "\t 6 occurs " << set_int.count(6)
          << " time(s)." << std::endl;
```

The output is

```
The set has 14 items.
         They are:   0  2  3  4  6  8  9 10 12 14 15 16 18 20
         6 occurs 1 time.
```

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END OF PART 5

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Start of ...

PART 6: `vector`

Part 6: vector

To use vector, we must

```
#include <vector>
```

Unlike a set, we can access a vector by index. Moreover, by default it is not sorted, though there are algorithms to sort its contents.

Since it is unordered, a new item usually gets added to the end, using push_back

This can be removed, using pop_back

Other important methods include

- at
- operator[]
- back (not the same as end)

Part 6: vector

03STL_vector.cpp

```
#include <vector>         // vector
#include <algorithm>      // sort
void print_int (int i) { std::cout << std::setw(3) << i; }
int main(void )
{
  std::vector <int> vec_int;
  std::vector <int>::iterator vec_int_i;
  std::cout << "Vector has " << vec_int.size() <<
    " elements." << std::endl ;

  for (int i=3; i>=0; i--)
    vec_int.push_back(i*3); // (9,6,3,0)

  std::cout << "Vector has " << vec_int.size() << " elements: ";
  for (unsigned int i=0; i<vec_int.size(); i++)
    std::cout << std::setw(3) << vec_int[i];
```

Output (so far):

```
Vector has 0 elements.
Vector has 4 elements:   9  6  3  0
```

Part 6: vector

This snippet demonstrates the use of

- the find and insert methods;
- the for_each iterate through an entire container.

03STL_vector.cpp

```
  vec_int_i = find (vec_int.begin(),vec_int.end(),3);
  vec_int.insert(vec_int_i ,10);

  std::cout << std::endl;
  std::cout << "Vector has " << vec_int.size() << " elements: ";
  for_each (vec_int.begin(), vec_int.end(), print_int);
```

Output (continued):

```
Vector has 0 elements.
Vector has 4 elements:   9  6  3  0
Vector has 5 elements:   9  6 10  3  0
```

Part 6: vector

Finally, we show how to sort the items in the list:

03STL_vector.h

```
  std::cout << "Sorting the vector..." << std::endl;
  sort(vec_int.begin(), vec_int.end());
  std::cout << "Now vector is: ";
  for_each (vec_int.begin(), vec_int.end(), print_int);
```

Output (all):

```
Vector has 0 elements.
Vector has 4 elements:    9   6   3   0
Vector has 5 elements:    9   6  10   3   0
Sorting the vector...
Now vector is:    0   3   6   9  10
```

Other `vector` methods

Other important methods include

- `begin()` (returns an iterator that points to the first element)
- `end()` (returns an iterator that points to *one past* the end of the set).
- `clear()` (remove contents)
- `count()` (count number of occuences)
- `empty()` (is the set empty?)
- `erase()` (remove an element, or range of elements)
- `find()` (locate an element; return an iterator)
- `size()` (number of elements)
- `swap()` (swap contents of two sets of same type)
- `for_each()` (apply a particular function to each item in a container)

Range-based for loops

The **ranged-based** *for* loop is a recent addition to C++, so it might not work with old compilers. With g++, you may need to enable the `c++11` option.

In the code above, the line

```
   for_each (vec_int.begin(), vec_int.end(), print_int);
```

could be replaced with

```
   for (int i : vec_int)
      print_int(i);
```

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END OF PART 6

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Start of ...

PART 7: **Algorithm**

Part 7: Algorithm

To use algorithm, we must

```
#include <algorithm>
```

Useful functions that this provides include

- for_each
- sort and partial_sort
- search
- copy and fill
- merge
- set_union, set_difference
- etc.

Part 7: Algorithm — The password frequency problem

(See lecture notes for details)

```
#include <set>       // multiset
#include <vector>    // vector
#include <algorithm> // sort
```

The password frequency problem

```
class pwd {
private:
  std::string word;
  int freq;
public:
  pwd(std::string s, int f) {word=s; freq=f;};
  std::string getword(void) const {return(word);};
  int getfreq(void) const {return(freq);};
};

bool compare (pwd p, pwd q)
{
  return (p.getfreq() > q.getfreq());
}

int FileLength(std::ifstream &InFile, int &LongestWord);
int main(void )
{
  std::ifstream InFile;
  std::string InFileName="UserAccount-1e5.txt";
  std::multiset <std::string> multi_pwd;
  std::multiset <std::string>::iterator multi_pwd_i;
  std::vector <pwd> vector_pwd;

  InFile.open(InFileName.c_str());
  if (InFile.fail() )
  {
    std::cerr << "Error: Cannot open " << InFileName <<
      " for reading." << std::endl;
    exit(1);
  }

  // Need to know the number of lines, and the length of the longest one
  int LineCount=0, LongestLine;
  LineCount =  FileLength(InFile, LongestLine);
  std::cout  << InFileName << " has " << LineCount << " lines.\n";
  std::cout  << "\tThe longest has " << LongestLine << " characters.\n";
```

The password frequency problem

```
// Read the lines
char *c_string_word;
c_string_word = new char [LongestLine+1];
for (int i=0; i<LineCount; i++)
{
  InFile.getline(c_string_word, LongestLine+1);
  multi_pwd.insert(c_string_word);
}
```

```
// Copy the passwords to the pwd vector
multi_pwd_i = multi_pwd.begin();
vector_pwd.push_back(pwd(*multi_pwd_i,
      multi_pwd.count(*multi_pwd_i)));
multi_pwd_i++;
while (multi_pwd_i != multi_pwd.end())
{
  if ((vector_pwd.back()).getword() != *multi_pwd_i)
    vector_pwd.push_back(pwd(*multi_pwd_i,
       multi_pwd.count(*multi_pwd_i)));
  multi_pwd_i++;
}
```

The password frequency problem

```
  std::sort (vector_pwd.begin(), vector_pwd.end(), compare);

  std::cout << "Top 10 passwords are: " << std::endl;
  for (unsigned int i=0; i<10; i++)
    std::cout <<  std::setw(12) << (vector_pwd[i]).getword() <<
      std::setw(6) << (vector_pwd[i]).getfreq() << std::endl;

  InFile.close();

  return(0);
}
```