## CS472/CM472/CS672 - Fall 2007: Assignment 1

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Due: Tuesday, October 2nd (at the beginning of class)

The main objective of this assignment is to familiarize yourself with the ia-ja data structures. The matrix of interest is the 2D Laplacian arising from heat flow problems. You should find this assignment fairly straightforward.

A model of heat flow is given by

$$
q_{x}=-\frac{\partial T}{\partial x}, \quad q_{y}=-\frac{\partial T}{\partial y},
$$

where $\left(q_{x}, q_{y}\right)$ is the heat flow velocity, and $T=T(x, y)$ is the temperature which satisfies the Poisson equation

$$
-\frac{\partial^{2} T}{\partial x^{2}}-\frac{\partial^{2} T}{\partial y^{2}}=f(x, y)
$$

Here, $f(x, y)$ is the heat source function.
We approximate the temperature function $T(x, y)$ at discrete locations on a two dimensional grid. Let the $(i, j)$ grid point have location $\left(x_{i}, y_{j}\right)$ where $x_{i}=i h, y_{j}=j h$, and $h=1 /(n+1)$ is the grid size. Let $T_{i, j} \approx T\left(x_{i}, y_{j}\right)$. Then the finite difference approximation results in a set of linear equations

$$
\begin{equation*}
\frac{1}{h^{2}}\left(4 T_{i, j}-T_{i-1, j}-T_{i+1, j}-T_{i, j-1}-T_{i, j+1}\right)=f_{i, j} . \tag{1}
\end{equation*}
$$

Solve (1) on an $n \times n$ grid with $i=1, \ldots, n ; j=1, \ldots, n$. (Note: we assume the boundary temperature at the sides of the grid are zero.) We want to analyze the heat flow with multiple central heating systems as shown in Figure 1; i.e.

$$
f_{i, j}=\left\{\begin{array}{lll}
1 & \text { if } & \left\|\left(x_{i}, y_{j}\right)-(0.25,0.25)\right\|_{2} \leq 0.1 \\
1 & \text { if } & \left\|\left(x_{i}, y_{j}\right)-(0.25,0.75)\right\|_{2} \leq 0.1 \\
1 & \text { if } & \left\|\left(x_{i}, y_{j}\right)-(0.75,0.25)\right\|_{2} \leq 0.1 \\
1 & \text { if } & \left\|\left(x_{i}, y_{j}\right)-(0.75,0.75)\right\|_{2} \leq 0.1 \\
0 & \text { otherwise. }
\end{array}\right.
$$

Define a vector $x$ such that

$$
x_{k}=T_{i, j},
$$

where $k=(j-1) * n+i$. Similarly, we define the vector $b$ with $b_{k}=f_{i, j}$. Then we can write equation (1) in the matrix form

$$
A x=b .
$$

The coefficient matrix $A$ is sparse of size $N \times N$, where $N=n^{2}$.


Figure 1: (a) Temperature function (b) Heat flow with four heat sources.

1. (10 marks) Set up the matrix $A$ and the right-hand side (RHS) $b$. Use ia-ja data structure for $A$ and an 1D array (i.e. full vector) for $b$. The main program, main.c, can be downloaded from the class homepage. It allocates appropriate memory for the arrays ia, ja and a as well as the RHS array b. Then it calls the functions matrix and source to set up the values for $A$ and $b$, respectively. Your job is to complete the body of these functions in the file matrhs.c. (Note: in C, indices start from 0 .)
In order to black box test your code, place your version of matrhs.c, matrhs.h in a single directory (nothing else in this directory) with the name
```
your_userid_your_student_id
```

Then zip up this directory using

```
zip -r your_userid_your_student_id your_userid_your_student_id
```

Mail the file

```
your_userid_your_student_id.zip
```

(as an attachment) to z4chen@cs.uwaterloo.ca. Your code will be tested by linking your code with the main.c calling routine (main.o), and running some tests. Submit a hard copy listing of the code as well.
2. (4 marks) To test your code, for the case $n=50$, uncomment the part of the code marked "Dump data" in main.c. (Note: it automatically converts the index range from 0 to $N-1$ in C to 1 to $N$ in MATLAB.) It will then save all data to the file output.m. The MATLAB program heatflow.m reads the data from output.m, solves the matrix equations and finally displays the temperature and heat flow of your computed solution. Submit the plots.
3. (6 marks) In a modified heat equation, the finite difference approximation results in a set of linear equations:
$\alpha T_{i-1, j-1}+\beta T_{i, j-1}+\gamma T_{i+1, j-1}+\mu T_{i-1, j}+\delta T_{i, j}+\nu T_{i+1, j}+\rho T_{i-1, j+1}+\eta T_{i, j+1}+\theta T_{i+1, j+1}=f_{i, j}$.
Let $A$ be the matrix of the linear system. Describe the sparsity structure of $A$ and the nonzero entries.
4. (6 marks) Consider solving the linear system: $A x=b$ where

$$
A=\left[\begin{array}{cccc}
1 & 1 & 0 & 3 \\
2 & 1 & -1 & 1 \\
3 & -1 & -1 & 2 \\
-1 & 2 & 3 & -1
\end{array}\right], \quad b=\left[\begin{array}{c}
4 \\
1 \\
-3 \\
4
\end{array}\right] .
$$

Let $L, U$ be the LU factorization of $A$, and $[\mathrm{L} \backslash \mathrm{U}]$ be the matrix whose upper triangular part is $U$ and lower triangular part is the same as the lower traingular part of $L$.
(a) Compute the $[\mathrm{L} \backslash \mathrm{U}]$ matrix using the standard Gaussian elimination. Show all your steps.
(b) Compute the $[\mathrm{L} \backslash \mathrm{U}]$ matrix using the Doolittle algorithm. Show all your steps.
(c) Using the $L, U$ factors computed from (a) (or (b)), compute the solution $x$.
5. (8 marks) Given a dense symmetric matrix $a_{i j}=a_{j i}$, we need only store the upper triangular part of $A$, i.e.

$$
\operatorname{Upper}(A)=a_{i j} j \geq i .
$$

It is desired to factor this matrix so that

$$
A=L U
$$

where $L$ is unit lower triangular. Give precise pseudo code for converting an upper triangular row $i$ of $A$ into row $i$ of $U$ (Doolittle form). For simplicity you may assume $A$ and $U$ are stored in separate matrices. This algorithm should operate only on the upper triangular part of $A$. (Hint: modify the pseudo code given in class for the Doolittle algorithm.) Then, give precise pseudo code (e.g., pseudo code for forward solve and backward solve) for solving

$$
L U x=b,
$$

by using only elements of $U$. (Hint: for symmetric $A$, we can factor $A=L D L^{T}$, where $L=$ lower triangular, unit diagonal and $D=$ diagonal. Thus $U=D L^{T}$, or equivalently, $L=$ $U^{T} D^{-1}$.)
6. (10 marks) Graduate student question. Suppose we have an ia-ja representation of the nonzero structure of a matrix having symmetric structure. However, the list for each row is unsorted. Assuming the number of nonzeros, $n n z(A)=O(N)$, describe an algorithm for sorting each of these lists in worst case complexity $O(N)$. Note that there is no $O(N \log N)$ term in this complexity, even if there is a dense row.

Hint: Let $C_{i}$ be the set of unsorted column indices for row $i$. Let $C_{i}^{\text {sorted }}$ be the sorted column indices for row $i$. Given $C_{i}, i=1, \ldots, N$, then we can construct $C_{i}^{\text {sorted }}, i=1, \ldots, N$ in the following way. Allocate $C_{i}^{\text {sorted }}$ of the correct size, $i=1, \ldots, N$. Then scan through the rows in the order $i=1, \ldots, N$. At row $i$, if $j \in C_{i}$, add column index $i$ to $C_{j}^{\text {sorted }}$.
Implement the sorting algorithm. Submit a listing of your code, and the results of a small test case from question 1. Name the sorting subroutine as symsort with the following prototype:

```
symsort(int *ia, int *ja, double *a, int N).
```

Include it in matrhs.c.

## Practice Problems (Do not hand in)

1. Show that if $A$ is diagonally dominant by rows, then so is $A^{(k)}$.
2. Describe an algorithm for computing the LU factorization of a matrix so that U is unit upper triangular.
3. The Minimum Degree strategy for determining an ordering of nodes for Gaussian Elimination is the following

- At each stage of the elimination, select the node which has the smallest degree (the degree of a node is the number of its graph neighbours). Ties are broken arbitrarily.

Given a matrix with symmetric structure, whose graph is a tree, use the graph model of Gaussian elimination to show that minimum degree ordering generates a perfect elimination sequence (no fill-in is produced).

