18.409 The Behavior of Algorithms in Practice	2/21/2002

Lecture 4

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A Gaussian Elimination Example

To solve:

$$\begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

First factor the matrix to get:

$$\begin{bmatrix} 1 & 0 \\ \frac{1}{\epsilon} & 1 \end{bmatrix} \begin{bmatrix} \epsilon & 1 \\ 0 & 1 - \frac{1}{\epsilon} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Next solve:

$$\begin{bmatrix} 1 & 0 \\ \frac{1}{\epsilon} & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

To get:

$$\begin{aligned} y_1 &= 1 \\ y_2 &= 1 - \frac{1}{\epsilon} \end{aligned}$$

Finally solve:

$$\begin{bmatrix} \epsilon & 1 \\ 0 & 1 - \frac{1}{\epsilon} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$$

To get:

$$\begin{aligned} x_1 &= 0 \\ x_2 &= 1 \end{aligned}$$

Which is the solution to the original system. When viewed this way, Gaussian elimination is just LU factorization of a matrix followed by some simple substitutions.

Floating Point

We consider a model of floating point computation where it is possible to represent numbers of the form:

$$\frac{m}{2^t}2^b$$

Where m is an integer such that $-2^t \leq m \leq 2^t$.

In this model, t is the precision of the floating point representation. In what follows, we will ignore bounds on b.

Let ϵ_{mach} be defined so that $1 + \epsilon_{mach}$ is the smallest number greater than 1 which the machine can represent.

The goal of a floating point computation is to provide an answer which is correct to within a factor of $(1 \pm \epsilon_{mach})$.

Consider the example in the previous section where $\epsilon < \epsilon_{mach}$. In this case, we will compute the LU factorization as:

$$\begin{bmatrix} 1 & 0 \\ \frac{1}{\epsilon} & 1 \end{bmatrix} \begin{bmatrix} \epsilon & 1 \\ 0 & -\frac{1}{\epsilon} \end{bmatrix}$$

This means that using Gaussian Elimination (with no pivoting) we will actually be solving the system:

$$\begin{bmatrix} \epsilon & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

And so will get the solution:

$$\begin{aligned} x_1 &= 1 \\ x_2 &= 1 - \epsilon \end{aligned}$$

Which is nowhere near the correct solution to the original system.

Note: The matrix in the previous example is well-conditioned, having a condition number of about 2.68, but we still fail miserably when doing Gaussian Elimination on this matrix.

Exercise: Do the same thing for the system:

$$\begin{bmatrix} 1 & 1 \\ \epsilon & 1 \end{bmatrix} \begin{bmatrix} x_2 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

You should observe that permuting the rows/columns of the matrix (pivoting) allows you to solve the system with Gaussian Elimination even when $\epsilon < \epsilon_{mach}$.

Theorem 1 (Wilkinson) *If you solve $Ax = b$ computing $\hat{L}$, $\hat{U}$ and $\hat{x}$, then there exists a δA such that*

$$(A + \delta A)\hat{x} = b$$

and

$$\frac{\|\delta A\|_\infty}{\|A\|_\infty} \leq n\epsilon_{mach}\left(3 + \frac{5\|\hat{L}\|_\infty\|\hat{U}\|_\infty}{\|A\|_\infty}\right)$$

The problem with the previous example is that although A had small entries, U had a very large entry.

When doing Gaussian Elimination, we say that the growth factor is:

$$\frac{\|U\|_\infty}{\|A\|_\infty}$$

Partial Pivoting

Idea: Permute the rows but not the columns such that the pivot is the largest entry in its column.

Note: This is the technique used by Matlab.

At step j in the Gaussian Elimination, permute the rows so that $|a_{j,j}| \geq |a_{i,j}|$ for all $i > j$.

This guarantees that $\|L\|_\infty \leq 1$. However, in the worst case, partial pivoting yields a growth factor of 2^{n-1} for an n-by-n matrix.

Complete Pivoting

Idea: Permute the rows and the columns such that the pivot is the largest entry in the matrix.

Wilkinson proved that Complete Pivoting guarantees that:

$$\frac{\|U\|_\infty}{\|A\|_\infty} \leq n^{\frac{1}{2}\log(n)}$$

However, it is conjectured that the growth factor can be upper bounded by something closer to n.

Unfortunately, using complete pivoting requires about twice as many floating point operations as partial pivoting. Therefore, since partial pivoting works well in practice, complete pivoting is hardly ever used.

Sometimes You Don't Need to Pivot

1. If A is diagonally dominant then it is possible to bound the size of the entries in L.

2. If A is positive definite then it is possible to bound the size of the entries in U.

Having both of these conditions is very nice. In practice, both of these conditions show up quite often.

Definition 2 *A matrix, A, is (column-wise) diagonally dominant if for all j,*

$$|a_{j,j}| \geq \sum_{i \neq j} a_{i,j}$$

Theorem 3 *If A is (column-wise) diagonally dominant, then $l_{i,j} \leq 1$. Equivalently, if A is diagonally dominant then one does not permute when using partial pivoting.*

Proof After the k^{th} round of Gaussian Elimination, we refer to the $n-k$ by $n-k$ matrix in the lower left corner as $A^{(k)}$.

If suffices to prove that all of the $A^{(k)}$ are diagonally dominant. We will show that $A^{(1)}$ is diagonally dominant. A straightforward inductive argument can be used to show all of the $A^{(k)}$ are diagonally dominant.

Claim 4 $A^{(1)}$ *is diagonally dominant.*

Let

$$A = \begin{bmatrix} \alpha & w \\ v & B \end{bmatrix}$$

Then one step of Gaussian Elimination yields

$$A = \begin{bmatrix} 1 & 0 \\ \frac{v}{\alpha} & I \end{bmatrix} \begin{bmatrix} \alpha & w \\ 0 & B - \frac{vw}{\alpha} \end{bmatrix}$$

Therefore, $A^{(1)} = B - \frac{vw}{\alpha}$.

Let $a^{(1)}_{i,j}$ be the i, j entry of $A^{(1)}$. It suffices to show that

$$|a^{(1)}_{j,j} \geq \sum_{i\geq 2, i\neq j} |a^{(1)}_{i,j}|$$

We know that

$$\sum_{i\geq 2, i\neq j} |a^{(1)}_{i,j}| = \sum_{i\geq 2, i\neq j} |b_{i,j} - \frac{v_i w_j}{\alpha}| \leq \sum_{i\geq 2, i\neq j} |b_{i,j}| + \frac{|w_j|}{\alpha} \sum_{i\geq 2, i\neq j} |v_i|$$

Since A is diagonally dominant, it follows that

$$\begin{aligned}
\sum_{i\geq 2, i\neq j} |a^{(1)}_{i,j}| &\leq (|b_{j,j}| - |w_j|) + \frac{|w_j|}{\alpha}(|\alpha| - |v_j|) = |b_{j,j}| - \frac{|w_j|}{|\alpha|}|v_j| \\
&\leq \left| b_{j,j} - \frac{w_j v_j}{\alpha} \right| = |a^{(1)}_{j,j}
\end{aligned}$$

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Definition 5 *A is positive definite if A is symmetric and for all x, $xAx^T > 0$*

Exercise: The above definition is equivalent to the following:

1. All eigenvalues of A are positive.
2. All principal minors of A are positive definite.

Exercise: Eigenvalues of $A_{2..n,2..n}$ interlace the eigenvalues of A.

Additionally, the following two facts are implied by Item #2 above:

- Diagonal entries of A are positive.
- The entry with the largest absolute value lies on a diagonal.

Theorem 6 *If A is positive definite, then $\|A^{(k)}\|_\infty \leq \|A\|_\infty$.*

Note: This implies that $\|U\|_\infty \leq \|A\|_\infty$.

Proof We first prove that the $A^{(k)}$ are positive definite. We will show that $A^{(1)}$ is positive definite. A straightforward inductive argument can be used to show all of the $A^{(k)}$ are diagonally dominant.

It is easy to see that $A^{(1)}$ is symmetric and so it suffices to show that for all x, $xAx^T > 0$.

Let

$$A = \begin{bmatrix} \alpha & v^T \\ v & B \end{bmatrix}$$

and recall that

$$A^{(1)} = B - \frac{vv^T}{\alpha}$$

Therefore,

$$xAx^T - (x_2 \ldots x_n)A^{(1)}(x_2 \ldots x_n)^T = \\ \alpha x_1^2 + 2x_1 \sum_{i \geq 2} v_i x_i + \sum_{i \geq 2, j \geq 2} b_{i,j} x_i x_j - \sum_{i \geq 2, j \geq 2} (b_{i,j} - \frac{v_i v_j}{\alpha}) x_i x_j$$

Therefore, by cancellation,

$$xAx^T - (x_2 \ldots x_n)A^{(1)}(x_2 \ldots x_n)^T = \alpha \left(x_i + \sum_{i \geq 2} \frac{v_i x_i}{\alpha} \right)^2$$

This means that for any $x_2 \ldots x_n$, setting

$$x_1 = -\sum_{i \geq 2} \frac{v_i x_i}{\alpha}$$

yields $xAx^T = (x_2 \ldots x_n)A^{(1)}(x_2 \ldots x_n)^T$. Therefore, if $A^{(1)}$ is not positive definite, then neither is A.

Now all that remains to be shown is that $\|A^{(1)}\|_\infty \leq \|A\|_\infty$. This will follow from two facts that were previously observed about positive definite matrices. (We repeat them here for convenience.

- Diagonal entries of A are positive.
- The entry with the largest absolute value lies on a diagonal.

Therefore, we know that the largest entry of $A^{(1)}$ is $a_{j,j}^{(1)}$ for some $j \geq 2$.

$$0 < a_{j,j}^{(1)} = b_{j,j} - \frac{v_j^2}{\alpha} \leq b_{j,j} = a_{j,j}$$

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A Smoothed Analysis Theorem

Theorem 7 *Let $\bar{A}$ be any matrix with $\|\bar{A}\|_\infty \leq 1$ and let $A = \bar{A} + G$ where G is a Gaussian random matrix with variance σ^2. Then*

$$Prob[\|U\|_\infty > 4n^{\frac{7}{2}}\sqrt{\log(n)}/\epsilon] < \frac{\epsilon}{\sigma} \tag{1}$$

$$Prob[\|L\|_\infty > 4n^{\frac{7}{2}}\sqrt{\log(n)}/\epsilon] < \frac{\epsilon\log(\frac{1}{\epsilon})}{\sigma} \tag{2}$$

where $A = LU$.

We will prove this theorem during the next lecture.