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Chapter 5: Linear Systems: Direct Methods

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Slides for the book
A First Course in Numerical Methods (published by SIAM, 2011)
http://www.ec-securehost.com/SIAM/CS07.html

Goals of this chapter

- To learn practical methods to handle the most common problem in numerical computation;
- to get familiar (again) with the ancient method of Gaussian elimination in its modern form of LU decomposition, and develop pivoting methods for its stable computation;
- to consider LU decomposition in the very important special cases of symmetric positive definite and sparse matrices;
- to study the expected quality of the computed solution, introducing as we go the fundamental concept of a condition number.

Outline

- Gaussian elimination and backward substitution
- LU decomposition
- Pivoting strategies
- Efficient implementation
- Cholesky decomposition
- Sparse matrices
- Permutations and ordering strategies
- Estimating error and the condition number

In general

- Here and in Chapter 7 we consider the problem of finding $\mathbf{x}$ which solves

  $$A\mathbf{x} = \mathbf{b},$$

  where A is a given, real, nonsingular, $n \times n$ matrix, and $\mathbf{b}$ is a given, real vector.
- *Such problems are ubiquitous in applications*!
- Two solution approaches:
  - *Direct methods*: yield exact solution in absence of roundoff error.
    - Variations of **Gaussian elimination**.
    - Considered in this chapter
  - *Iterative methods*: iterate in a similar fashion to what we do for nonlinear problems.
    - Use only when direct methods are ineffective.
    - Considered in Chapter 7

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Backward substitution

- Special case: A is an **upper triangular** matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ & a_{22} & \ddots & \vdots \\ & & \ddots & \vdots \\ & & & a_{nn} \end{pmatrix},$$

  i.e., all elements below the main diagonal are zero: $a_{ij} = 0, \forall i > j$.

- The algorithm:

$$\begin{aligned} &\text{for } k = n : -1 : 1 \\ &\quad x_k = \frac{b_k - \sum_{j=k+1}^{n} a_{kj} x_j}{a_{kk}} \\ &\text{end} \end{aligned}$$

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\end{aligned}$$

Example

$$\begin{aligned} x_1 - 4x_2 + 3x_3 &= -2 \\ 5x_2 - 3x_3 &= 7 \\ -2x_3 &= -2 \end{aligned}$$

In matrix form:

$$\begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -2 \\ 7 \\ -2 \end{pmatrix}.$$

Backward substitution: $x_3 = \frac{-2}{-2} = 1$, then $x_2 = \frac{1}{5}(7 + 3 \cdot 1) = 2$, then $x_1 = -2 + 4 \cdot 2 - 3 \cdot 1 = 3$.

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where all elements above the main diagonal are zero: $a_{ij} = 0, \forall i < j$.

- The algorithm:

$$\begin{array}{l} \text{for } k = 1 : n \\ \quad x_k = \dfrac{b_k - \sum_{j=1}^{k-1} a_{kj} x_j}{a_{kk}} \\ \text{end} \end{array}$$

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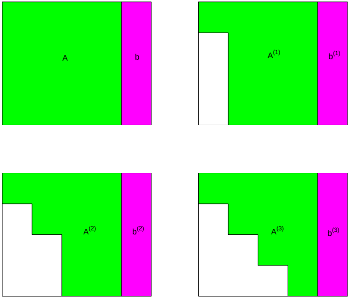
Gaussian elimination

- Can multiply a row of $A\mathbf{x} = \mathbf{b}$ by a scalar and add to another row: **elementary transformation**.
- Use this to transform A to upper triangular form:

$$MA\mathbf{x} = M\mathbf{b}, \quad U = MA.$$

- Apply backward substitution to solve $U\mathbf{x} = M\mathbf{b}$.



Gaussian elimination (basic)

for $k = 1 : n-1$

  for $i = k+1 : n$

    $l_{ik} = \dfrac{a_{ik}}{a_{kk}}$

    for $j = k+1 : n$

      $a_{ij} = a_{ij} - l_{ik} a_{kj}$

    end

    $b_i = b_i - l_{ik} b_k$

  end

end

Then apply backward substitution.

Note: upper part of A is overwritten by U, lower part no longer of interest.

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Cost (flop count)

- For the elimination:

$$\approx 2\sum_{k=1}^{n-1}(n-k)^2 = 2((n-1)^2 + (n-2)^2 + \cdots + 1^2) = \frac{2}{3}n^3 + \mathcal{O}(n^2).$$

- For the backward substitution:

$$\approx 2\sum_{k=1}^{n-1}(n-k) = 2\frac{(n-1)n}{2} \approx n^2.$$

Example

- Solve $A\mathbf{x} = \mathbf{b}$ for
$$A = \begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} -2 \\ 5 \\ 6 \end{pmatrix}.$$
- Gaussian elimination: $(A \mid \mathbf{b}) \Rightarrow$
$$\left(\begin{array}{ccc|c} 1 & -4 & 3 & -2 \\ 0 & 5 & -3 & 7 \\ 0 & 10 & -8 & 12 \end{array}\right) \Rightarrow \left(\begin{array}{ccc|c} 1 & -4 & 3 & -2 \\ 0 & 5 & -3 & 7 \\ 0 & 0 & -2 & -2 \end{array}\right).$$
- Backward substitution: $x_3 = \frac{-2}{-2} = 1$, then $x_2 = \frac{1}{5}(7 + 3 \cdot 1) = 2$, then $x_1 = -2 + 4 \cdot 2 - 3 \cdot 1 = 3$.

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LU decomposition

- What if we have many right hand side vectors, or we don't know $\mathbf{b}$ right away?
- Note that determining transformation M such that $MA = U$ does not depend on $\mathbf{b}$.
- $M = M^{(n-1)} \dots M^{(2)} M^{(1)}$, where $M^{(k)}$ is the transformation of the kth outer loop step. These are elementary lower triangular matrices, e.g.,

$$M^{(2)} = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & -l_{32} & \ddots & & \\ & \vdots & & \ddots & \\ & -l_{n2} & & & 1 \end{pmatrix}.$$

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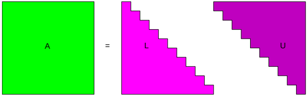
LU decomposition (cont.)

- The matrix M is unit lower triangular.
- The matrix $L = M^{-1}$ is also unit lower triangular:

$$A = LU, \quad L = \begin{pmatrix} 1 & & & & \\ l_{21} & 1 & & & \\ l_{31} & l_{32} & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ l_{n1} & l_{n2} & \cdots & l_{n,n-1} & 1 \end{pmatrix}.$$

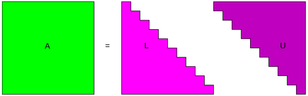
LU decomposition (cont.)



So, Gaussian elimination is equivalent to:

1. decompose $A = LU$.
   Now for a given $\mathbf{b}$ *we have to solve* $L(U\mathbf{x}) = \mathbf{b}$ *:*
2. use forward substitution to solve $L\mathbf{y} = \mathbf{b}$;
3. use backward substitution to solve $U\mathbf{x} = \mathbf{y}$.

LU decomposition (cont.)



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Example

$$A = \begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix}.$$

Obtain

1. $l_{21} = \frac{1}{1} = 1, \; l_{31} = \frac{3}{1} = 3$, so

$$M^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -3 & 0 & 1 \end{pmatrix}, \quad A^{(1)} = M^{(1)}A = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 10 & -8 \end{pmatrix}.$$

2. $l_{32} = \frac{10}{5} = 2$, so

$$M^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -2 & 1 \end{pmatrix}, \quad A^{(2)} = M^{(2)}A^{(1)} = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix}.$$

Example (cont.)

- We thus obtain

$$U = A^{(2)} = M^{(2)} A^{(1)} = \begin{pmatrix} 1 & -4 & 3 \\ 0 & 5 & -3 \\ 0 & 0 & -2 \end{pmatrix},$$

and collect the multipliers l_{21}, l_{31} and l_{32} into the unit lower triangular matrix

$$L = \begin{pmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 3 & 2 & 1 \end{pmatrix}.$$

- Indeed, $A = LU$:

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

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Examples where the LU decomposition is useful

- When we have multiple right-hand sides, form *once* the LU decomposition (which costs $\mathcal{O}(n^3)$ flops); then for each right-hand side only apply forward/backward substitutions (which are computationally cheap at $\mathcal{O}(n^2)$ flops each).
- Can compute A^{-1} by decomposing $A = LU$ once, and then solving $LU\mathbf{x} = \mathbf{e}_k$ for each column $\mathbf{e}_k$ of the unit matrix. These are n right hand sides, so the cost is approximately $\frac{2}{3}n^3 + n \cdot 2n^2 = \frac{8}{3}n^3$ flops. (However, typically we try to avoid computing the inverse A^{-1}; the need to compute it *explicitly* is rare.)
- Compute determinant of A by

$$\det(A) = \det(L)\det(U) = \Pi_{k=1}^{n} u_{kk}.$$

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Example: need for pivoting

- First step of Gaussion elimination:

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 1 & 2 & 2 \\ 1 & 2 & 2 & 3 \end{array}\right) \Rightarrow \left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 2 \end{array}\right).$$

- Second step: Now $a_{22}^{(1)} = 0$ and we're stuck.
- Simple remedy: exchange rows 2 and 3:

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 3 \\ 1 & 1 & 2 & 2 \end{array}\right) \Rightarrow \left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 2 \\ 0 & 0 & 1 & 1 \end{array}\right).$$

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Partial pivoting

- It is rare to hit precisely a zero pivot, but common to hit a very small one.
- Example:

$$\left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 1 & 1+10^{-12} & 2 & 2 \\ 1 & 2 & 2 & 3 \end{array}\right) \Rightarrow \left(\begin{array}{ccc|c} 1 & 1 & 1 & 1 \\ 0 & 10^{-12} & 1 & 1 \\ 0 & 1 & 1 & 2 \end{array}\right).$$

- Now we get a multplier $l_{3,2} = 1/10^{-12} = 10^{12}$, so roundoff error in elimination step is magnified by this factor 10^{12}.
- Employ Gaussian elimination with partial pivoting (GEPP) not just to avoid zero pivots but more generally to obtain a *stable* algorithm.

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GEPP

- At each stage k choose $q = q(k)$ as the smallest integer for which

$$|a_{qk}^{(k-1)}| = \max_{k \le i \le n} |a_{ik}^{(k-1)}|,$$

and interchange rows k and q.

- This ensures that pivots are not too small (unless matrix is close to singular) and $|l_{i,k}| \le 1, \text{ all } i \ge k$.
- $PA = LU$ where P is permutation matrix, e.g.,

$$P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

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Simple GEPP algorithm

for $k = 1 : n-1$

  for $i = k+1 : n$

    $q = \arg \max_{k \le i \le n} |a_{ik}^{(k-1)}|$

    exchange rows k and q

    $l_{ik} = \dfrac{a_{ik}}{a_{kk}}$

    for $j = k+1 : n$

      $a_{ij} = a_{ij} - l_{ik} * a_{kj}$

    end

    $b_i = b_i - l_{ik} * b_k$

  end

end

Forming $PA = LU$

- It's not so obvious, but it's true, that with

$$B = M^{(n-1)}P^{(n-1)} \cdots M^{(2)}P^{(2)}M^{(1)}P^{(1)}, \quad P = P^{(n-1)} \cdots P^{(2)}P^{(1)},$$

we get L lower triangular and

$$B = L^{-1}P.$$

- The matrix L is lower triangular, although not the same as it would be without pivoting. It is obtained by a similar sequence of steps as before, with the addition of permutation steps.
- The permutation matrix P is orthogonal, so

$$A = (P^T L)U.$$

$P^T L$ is "psychologically lower triangular".
In practice, keep record of permutations in a 1D array.

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Example revisited (1/3)

Same matrix we worked on a few slides ago, now with pivoting:

$$A = \begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix}.$$

Go through first column and find pivot:

$$P^{(1)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \;;\; P^{(1)}A = \begin{pmatrix} 3 & -2 & 1 \\ 1 & 1 & 0 \\ 1 & -4 & 3 \end{pmatrix}.$$

So, we have

$$M^{(1)} = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{1}{3} & 1 & 0 \\ -\frac{1}{3} & 0 & 1 \end{pmatrix}, \;\; A^{(1)} = M^{(1)}P^{(1)}A = \begin{pmatrix} 3 & -2 & 1 \\ 0 & \frac{5}{3} & -\frac{1}{3} \\ 0 & -\frac{10}{3} & \frac{8}{3} \end{pmatrix}.$$

Example revisited (2/3)

Now, work on $A^{(1)}$:

$$P^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \; ; \;\; P^{(2)}A^{(1)} = \begin{pmatrix} 3 & -2 & 1 \\ 0 & -\frac{10}{3} & \frac{8}{3} \\ 0 & \frac{5}{3} & -\frac{1}{3} \end{pmatrix},$$

and we have

$$M^{(2)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & \frac{1}{2} & 1 \end{pmatrix}, \;\; A^{(2)} = M^{(2)}P^{(2)}M^{(1)}P^{(1)}A = \begin{pmatrix} 3 & -2 & 1 \\ 0 & -\frac{10}{3} & \frac{8}{3} \\ 0 & 0 & 1 \end{pmatrix}.$$

So the upper triangular U is $U = A^{(2)} = M^{(2)}P^{(2)}M^{(1)}P^{(1)}A$.

Example revisited (3/3)

- Let us find L and P. Write

$$U = M^{(2)}P^{(2)}M^{(1)}P^{(1)}A = \underbrace{\left(M^{(2)}\right)}_{\tilde{M}^{(2)}}\underbrace{\left(P^{(2)}M^{(1)}{P^{(2)}}^T\right)}_{\tilde{M}^{(1)}}\underbrace{\left(P^{(2)}P^{(1)}\right)}_{P}A.$$

- Next, take the elements of L below the diagonal to be those of the $\tilde{M}^{(k)}$ with flipped signs; the permutation matrix P is just the product of the $P^{(k)}$:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \frac{1}{3} & -\frac{1}{2} & 1 \end{pmatrix}; \quad U = \begin{pmatrix} 3 & -2 & 1 \\ 0 & -\frac{10}{3} & \frac{8}{3} \\ 0 & 0 & 1 \end{pmatrix}; \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

  Exercise: confirm that indeed, $PA = LU$.

- In MATLAB obtain these matrices by the commands
```
A=[1 -4 3; 1 1 0; 3 -2 1];
[L,U,P]=lu(A);
```
- For more on the general principle illustrated in this example, see pages 107–108 in the book, as well as Exercises 7 and 8 of Chapter 5.

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- Let us find L and P. Write

$$U = M^{(2)}P^{(2)}M^{(1)}P^{(1)}A = \underbrace{\left(M^{(2)}\right)}_{\tilde{M}^{(2)}}\underbrace{\left(P^{(2)}M^{(1)}{P^{(2)}}^T\right)}_{\tilde{M}^{(1)}}\underbrace{\left(P^{(2)}P^{(1)}\right)}_{P}A.$$

- Next, take the elements of L below the diagonal to be those of the $\tilde{M}^{(k)}$ with flipped signs; the permutation matrix P is just the product of the $P^{(k)}$:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{3} & 1 & 0 \\ \frac{1}{3} & -\frac{1}{2} & 1 \end{pmatrix}; \quad U = \begin{pmatrix} 3 & -2 & 1 \\ 0 & -\frac{10}{3} & \frac{8}{3} \\ 0 & 0 & 1 \end{pmatrix}; \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

  Exercise: confirm that indeed, $PA = LU$.

- In MATLAB obtain these matrices by the commands

```
A=[1 -4 3; 1 1 0; 3 -2 1];
[L,U,P]=lu(A);
```

- For more on the general principle illustrated in this example, see pages 107–108 in the book, as well as Exercises 7 and 8 of Chapter 5.

GEPP stability

- Want to be assured that

$$g_n(A) = \max_{i,j,k} |a_{i,j}^{(k)}|$$

does not grow exponentially in n. However, this is easily said than done!

- Bad scaling of rows can fool the GEPP we saw, because multiplying a row of $(A \mid \mathbf{b})$ by an arbitrary nonzero constant can affect which $q = k$ maximizes $|a_{ik}^{(k-1)}|$.
- Can occasionally do better by **scaled partial pivoting**, where pivot dominance is relative to its original row norm.
- However, *provably* stable is only the more expensive **complete pivoting**. And yet, in practice partial pivoting is usually sufficient.
- There are special cases where no pivoting is required, including symmetric positive definite and disagonally dominant matrices.

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GEPP vectorization

- Memory access and inter-processor communications can be as expensive as floating point operations.
- A simple way to improve efficiency in MATLAB is to avoid *if*- *for*- and *while*-loops where possible.
- Work with array operations rather than on individual elements.

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for k = 1:n-1
  % find pivot q [...]
  % interchange rows k and q and record this in p
  A([k,q],:)=A([q,k],:);   p([k,q])=p([q,k]);
  % compute the corresponding column of L
  J=k+1:n; A(J,k) = A(J,k) / A(k,k);
  % update submatrix by outer product
  A(J,J) = A(J,J) - A(J,k) * A(k,J);
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Inner and outer products

Example:

$$\mathbf{y} = \begin{pmatrix} 3 \\ 2 \\ 1 \end{pmatrix}, \quad \mathbf{z} = \begin{pmatrix} 0 \\ 1 \\ 3 \end{pmatrix}.$$

- Inner product

$$\mathbf{y}^T\mathbf{z} = \mathbf{z}^T\mathbf{y} = 3*0 + 2*1 + 1*3 = 5.$$

- Outer products

$$\mathbf{y}\mathbf{z}^T = \begin{pmatrix} 0 & 3 & 9 \\ 0 & 2 & 6 \\ 0 & 1 & 3 \end{pmatrix}, \quad \mathbf{z}\mathbf{y}^T = \begin{pmatrix} 0 & 0 & 0 \\ 3 & 2 & 1 \\ 9 & 6 & 3 \end{pmatrix}.$$

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Example

Same matrix as before, now with vectorized GEPP:

$$A = \begin{pmatrix} 1 & -4 & 3 \\ 1 & 1 & 0 \\ 3 & -2 & 1 \end{pmatrix}.$$

Obtain for the first column $k = 1$ without pivoting

1. $J = [2,3]$, $A([2,3],1) = \begin{pmatrix} 1 \\ 3 \end{pmatrix}$, $A(1,[2,3]) = \begin{pmatrix} -4 & 3 \end{pmatrix}$, so the upate is
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Fast memory access and BLAS

- Computer memories are built as *hierarchies*: from faster, smaller and more expensive to slower, larger and cheaper.
    1. registers
    2. cache
    3. memory
    4. disk, cloud
- Standardize basic matrix operations into BLAS:
    1. BLAS1: $a * \mathbf{x} + \mathbf{y}$ (SAXPY)
    2. BLAS2: matrix-vector operations
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The "square root" of a symmetric positive definite matrix

- Recall that symmetric positive definite is the concept extension of a positive scalar to square real matrices A.
- For a scalar $a > 0$ there is a real square root, i.e., a real scalar g s.t. $g^2 = a$.
- For a symmetric positive matrix A, the Cholesky decomposition is written as

$$A = GG^T$$

where G is a *lower triangular matrix*.
- Obtain Cholesky as a special case of LU decomposition, utilizing both symmetry of A and the assurance that no partial pivoting is needed.

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Cholesky decomposition

- Since A is symmetric positive definite, we can stably write

  $$A = LU.$$

- Factor out the diagonal of U

$$U = \begin{pmatrix} u_{11} & & & & \\ & u_{22} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & u_{nn} \end{pmatrix} \begin{pmatrix} 1 & \frac{u_{12}}{u_{11}} & \cdots & \cdots & \frac{u_{1n}}{u_{11}} \\ & 1 & \frac{u_{23}}{u_{22}} & \cdots & \frac{u_{2n}}{u_{22}} \\ & & \ddots & & \vdots \\ & & & \ddots & \vdots \\ & & & & 1 \end{pmatrix} = D\tilde{U}.$$

- So $A = LD\tilde{U}$, and by symmetry, $A = LDL^T$.

Cholesky decomposition cont.

- By an elementary linear algebra theorem, $u_{kk} > 0$, $k = 1, \ldots, n$, so can define

$$D^{1/2} = diag\{\sqrt{u_{11}}, \ldots, \sqrt{u_{nn}}\}.$$

- Obtain $A = GG^T$ with $G = LD^{1/2}$.
- Compute directly, using symmetry, in $\frac{1}{3}n^3 + \mathcal{O}(n^2)$ flops.
- In MATLAB, `R = chol(A)` gives $R = G^T$.

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Cholesky Algorithm

Given a symmetric positive definite $n \times n$ matrix A, this algorithm overwrites its lower part with its Cholesky factor.

$$
\begin{aligned}
&\text{for } k = 1 : n \\
&\quad a_{kk} = \sqrt{a_{kk}} \\
&\quad \text{for } i = k+1 : n \\
&\quad\quad a_{ik} = \frac{a_{ik}}{a_{kk}} \\
&\quad \text{end} \\
&\quad \text{for } j = k+1 : n \\
&\quad\quad \text{for } i = j : n \\
&\quad\quad\quad a_{ij} = a_{ij} - a_{ik} a_{jk} \\
&\quad\quad \text{end} \\
&\quad \text{end} \\
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Sparse matrix

- Suppose A is $n \times n$ (although it can more generally be rectangular). The matrix is *sparse* if most its elements are zero: $\mathtt{nz} = m \ll n^2$.
- Think of a case where only $m = \mathcal{O}(n)$ elements are nonzero.
- Then convenient to represent by triplet form $(\mathbf{i}, \mathbf{j}, \mathbf{v})$, such that

$$v_k = a_{i_k, j_k} \quad k = 1, 2, \ldots, m.$$

- MATLAB has many special sparse matrix operations, e.g., `sparse`, `spdiags`: great for improved efficiency, not-so-great for code readability and friendliness.

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Banded matrices

- The simplest, most well-organized sparse matrix case is where all nonzeros of A are in a band of diagonals neighboring the main diagonal.

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1q} & & & & \\ \vdots & \ddots & \ddots & \ddots & & & \\ a_{p1} & \ddots & \ddots & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots & \ddots & a_{n-q+1,n} \\ & & & \ddots & \ddots & \ddots & \vdots \\ & & & & a_{n,n-p+1} & \cdots & a_{nn} \end{pmatrix}.$$

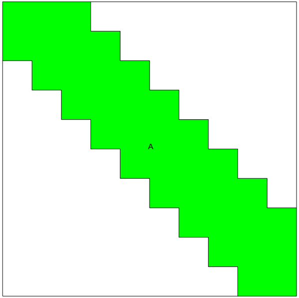
- So,

$$a_{ij} = 0, \text{ if } i \geq j + p, \text{ or if } j \geq i + q.$$

The **bandwidth** is $p + q - 1$.

Special banded matrices

- For a **diagonal** matrix, $p = q = 1$;
- for a full (or **dense**) matrix, $p = q = n$;
- for a tridiagonal matrix, $p = q = 2$.



GE (and LU decomposition) for banded matrices

for $k = 1 : n - 1$

for $i = k + 1 : k + p - 1$

$$l_{ik} = \frac{a_{ik}}{a_{kk}}$$

for $j = k + 1 : k + q - 1$

$$a_{ij} = a_{ij} - l_{ik} a_{kj}$$

end

$$b_i = b_i - l_{ik} b_k$$

end

end

Cost (flop count): if p and q are constant as n grows then cost is $\mathcal{O}(n)$, which is a major improvement over the dense matrix case.

GEPP for banded matrices

- Essentially the same algorithm as without pivoting. However:
- The upper bandwidth of U may increase from q to $q+p-1$.
- The matrix L, although it remains unit lower triangular, is no longer tightly banded (although it has the same number of nonzeros per column).

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Fill-in

- Consider solving

$$A\mathbf{x} = \mathbf{b}$$

where A is large and **sparse** (a vast majority of its elements are zero).
- Want to use GE (LU decomposition).
- But may have problem of **fill-in** during the elimination process, i.e., L and U together may have many more nonzero elements than A.
- Example: Arrow I

$$A = \begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & 0 & 0 & 0 \\ \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & \times & 0 \\ \times & 0 & 0 & 0 & \times \end{pmatrix}.$$

(Think of a symmetric matrix with $n = 500$, say.)
- Here both L and U could have completely full triangles: *disastrous fill-in*.

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Essentially no fill-in outside the band, but possible fill-in inside the band.

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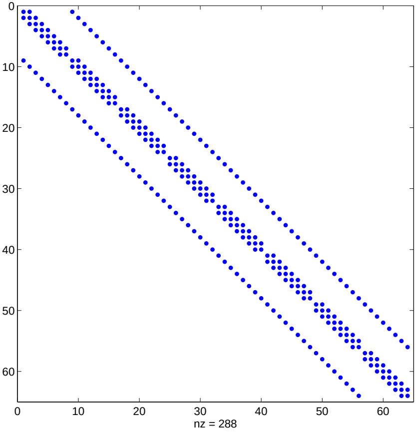
Example: model Poisson problem



The $2\sqrt{n}$ inner zero diagonals may be filled in upon using LU decomposition...

Permutations and ordering strategies

What can we do to obtain little or no fill-in?

- No perfect solution for this problem.
- Occasionally, permuting rows and columns of A significantly helps in reducing fill-in.
- Leads to considerations involving graph theory.
- Common goals are:
  - Reduce the bandwidth of the matrix; e.g., reverse Cuthill-McKee (RCM)
  - Reduce the expected fill-in in the decomposition stage; e.g., (approximate) minimum degree (AMD).

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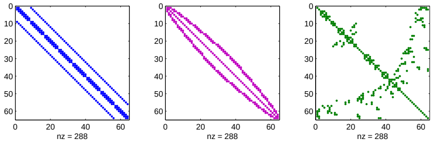
Now there is no fill-in upon applying LU decomposition.

2. Model Poisson problem



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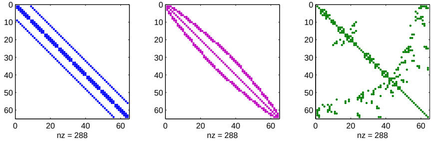

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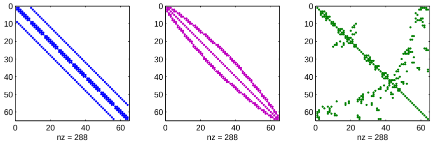

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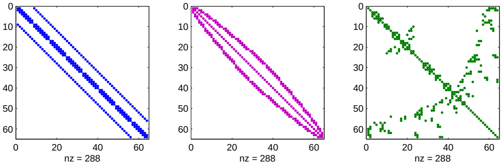
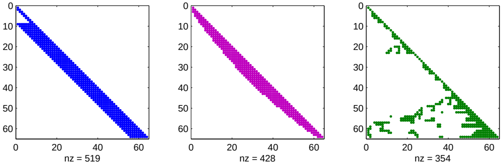
Example: fill-in for Poisson

- Permuted matrix patterns



- After Cholesky decomposition



Outline

- Gaussian elimination and backward substitution
- LU decomposition
- Pivoting strategies
- Efficient implementation
- Cholesky decomposition
- Sparse matrices
- Permutations and ordering strategies
- Estimating error and the condition number

Relative error in the solution

- Still consider

$$A\mathbf{x} = \mathbf{b}$$

but now assess quality of approximate solution obtained somehow.

- Denote exact solution $\mathbf{x}$, computed (or given) approximate solution $\hat{\mathbf{x}}$. Want to estimate

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|}.$$

- Can compute the residual $\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}}$ and so also $\frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|}$.
Does a small relative residual imply small relative error in solution?

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Example

- For the problem

$$A = \begin{pmatrix} 1.2969 & .8648 \\ .2161 & .1441 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} .8642 \\ .1440 \end{pmatrix},$$

  consider the approximate solution

$$\hat{\mathbf{x}} = \begin{pmatrix} .9911 \\ -.4870 \end{pmatrix}.$$

- Then

$$\hat{\mathbf{r}} = \mathbf{b} - A\hat{\mathbf{x}} = \begin{pmatrix} -10^{-8} \\ 10^{-8} \end{pmatrix},$$

  so $\|\hat{\mathbf{r}}\|_\infty = 10^{-8}$.

- However, the exact solution is

$$\mathbf{x} = \begin{pmatrix} 2 \\ -2 \end{pmatrix}, \quad \text{so} \quad \|\mathbf{x} - \hat{\mathbf{x}}\|_\infty = 1.513.$$

Conditioning of problem

- Since $\hat{\mathbf{r}} = A\mathbf{x} - A\hat{\mathbf{x}} = A(\mathbf{x} - \hat{\mathbf{x}})$, get

$$\|\mathbf{x} - \hat{\mathbf{x}}\| = \|A^{-1}\hat{\mathbf{r}}\| \leq \|A^{-1}\|\|\hat{\mathbf{r}}\|.$$

- Since $A\mathbf{x} = \mathbf{b}$, get

$$\frac{1}{\|\mathbf{x}\|} \leq \frac{\|A\|}{\|\mathbf{b}\|}.$$

- Hence

$$\begin{aligned} \frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} &\leq \kappa(A)\frac{\|\hat{\mathbf{r}}\|}{\|\mathbf{b}\|}, \\ \kappa(A) &= \|A\|\|A^{-1}\|. \end{aligned}$$

The scalar $\kappa(A)$ is the **condition number** of A.

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Quality of solution

- Backward error analysis: associate result of numerical algorithm (GEPP) with the **exact solution** of a **perturbed problem**

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

- The job of GEPP is to make δA and $\delta \mathbf{b}$ small.
- Obtain good quality solution (only) if in addition, $\kappa(A)$ is not too large.
- In our 2×2 example, in fact, $\kappa(A) \approx 10^8$, and indeed we saw $\|\mathbf{x} - \hat{\mathbf{x}}\| \sim \kappa(A)\|\hat{\mathbf{r}}\|$.

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The condition number

- Always $\kappa(A) \geq 1$.
- For orthogonal matrices, $\kappa_2(Q) = 1$: ideally conditioned!
- $\kappa(A)$ indicates how close A is to being singular, which $det(A)$ does not.
- If A is symmetric positive definite with eigenvalues $\lambda_1 \geq \cdots \geq \lambda_n > 0$ then

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