Computational Linear Algebra

- **Course:** (MATH: 6800, CSCI: 6800)
- **Semester:** Fall 1998
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References

1. O. Axelsson (1994), *Iterative Solution Methods*, Cambridge, Cambridge.

2. R. Barrett, M. Berry, T. Chan, J. Demmel, J. Donato, J. Dongarra, V. Eijkhout, V. Pozo, C. Romine, and H. van der Vorst (1994), *Templates for the Solution of Linear Systems: Building Blocks for Iterative Methods*, SIAM, Philadelphia.

3. Å. Björck (1996), *Numerical Methods for Least Squares Problems*, SIAM, Philadelphia.

4. W. Briggs (1987), *A Multigrid Tutorial*, SIAM, Philadelphia.

5. J.W. Demmel (1997), *Applied Numerical Linear Algebra*, SIAM, philadelphia.

6. A. George and J. Liu (1981), *Computer Solution of Large Sparse Positive Definite Systems*, Prentice-Hall, Englewood Cliffs.

7. G.H. Golub and C.F. Van Loan (1993), *Matrix Computations*, Third Edition, Johns Hopkins, Baltimore.

8. A. Greenbaum (1997), *Iterative Methods for Solving Linear Systems*, SIAM Philadelphia.

9. W. Hackbusch (1994), *Iterative Solution of Large Sparse Linear Systems of Equations*, Springer-Verlag, Berlin.

10. N. Higham (1996), *Accuracy and Stability of Numerical Algoritms*, SIAM Philadelphia.

11. B. Parlett (1980), *The Symmetric Eigenvalue Problem*, Prentice-Hall, Englewood Cliffs.

12. Y. Saad (1996), *Iterative Methods for Sparse Linear Systems*, PWS, Boston.

13. B. Smith, P. Bjorstad, and W. Gropp (1996), *Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations*, Cambridge, Cambridge.

14. G.W. Stewart (1973), *Introduction to Matrix Computations*, Academic Press, New York.

15. G.W. Stewart and J.-G. Sun (1990) *Matrix Perturbation Theory*, Academic Press, New York.

16. L.N. Trefethen and D. Bau, III (1997), *Numerical Linear Algebra*, SIAM, Philadelphia. [1]

17. P. Wesseling (1992), *An Introduction to Multigrid Methods*, Wiley, Chichester.

[1] Text

18. D. Young (1971), *Iterative Solution of Large Linear Systems*, Academic Press, New York.

1. Introduction

1.1. Notation

- *Motivation:*
  - Linear algebra is involved in approximately 75% of scientific computation
    - Circuit and network analysis
    - Potential theory
    - Signal processing
    - Acoustics and vibrations
    - Optimization
    - Finite difference and finite element methods
    - Tomography
    - Optimal control

- *Problems:*
  - Solve linear systems
  - Solve least squares problems
  - Solve eigenvalue-eigenvector problems

Notation

- Reading: Trefethen and Bau (1997), Lecture 1
- An $m \times n$ matrix

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \tag{1}$$

  - Bold letters denote vectors and matrices
  - Italic letters denote scalars
    - Lower case letters are elements of a matrix
  - $a_{ij} \in \Re$, $i = 1, 2, ..., m$, $j = 1, 2, ..., n$, unless stated
  - $\mathbf{A} \in \Re^{m \times n}$
    - $\Re^{m \times n}$ a vector space of $m \times n$ real matrices
  - A vector: $\mathbf{x} \in \Re^{m \times 1} := \Re^m$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}, \qquad \mathbf{x}^T = [x_1, x_2, \cdots, x_m]$$

MATLAB

- Specify Algorithms using *MATLAB*
- *Vector dot (scalar) product*

$$c = \mathbf{x}^T\mathbf{y} = \sum_{i=1}^{n} x_i y_i \tag{2}$$

function c = dot($\mathbf{x}$, $\mathbf{y}$)
% dot: compute a dot product of the n-vectors $\mathbf{x}$ and $\mathbf{y}$
  n = length($\mathbf{x}$)
  c = 0
  for i = 1:n
    c = c + x(i)*y(i)
  end

  - Subscripts are enclosed in parentheses
  - The MATLAB function *length* computes the dimension of a vector
  - The : indicates a range
    - In the for loop, i ranges over integers from 1 to n
  - dot($\mathbf{x}$, $\mathbf{y}$) is a library function in MATLAB

A SAXPY

- A *saxpy* ("scalar a x plus y") is the vector

$$\mathbf{z} = a\mathbf{x} + \mathbf{y} \tag{3}$$

function $\mathbf{z}$ = saxpy(a, $\mathbf{x}$, $\mathbf{y}$)
% saxpy: compute the vector $\mathbf{z}$ = a $*$ $\mathbf{x}$ + $\mathbf{y}$ where
% a is a scalar and $\mathbf{x}$ and $\mathbf{y}$ are vectors
  n = length($\mathbf{x}$)
  for i = 1:n
    z(i) = a*x(i) + y(i)
  end

  - $\mathbf{x}$ and $\mathbf{y}$ have the same dimensions n
    - Production software should check this

Matrix Multiplication

- Let $\mathbf{A} \in \Re^{m \times r}$, $\mathbf{B} \in \Re^{r \times n}$, and $\mathbf{C} \in \Re^{m \times n}$, then

$$c_{ij} = \sum_{k=1}^{r} a_{ik} b_{kj}, \qquad i = 1 : m, \qquad j = 1 : n \tag{4}$$

```
function C = matmy(A, B)
% matmy: compute the matrix product C = AB
   [m r] = size(A);
   [r n] = size(B);
   for i = 1:m
      for j = 1:n
         C(i,j) = 0;
         for k = 1:r
            C(i,j) = C(i,j) + A(i,k)*B(k,j);
         end
      end
   end
```

  - size(**A**) returns the row and column dimensions of **A**
  - The ;s suppress printing of results
  - The complexity is mnr multiplications and additions
  - Some details are omitted

Matrix Multiplication

- Matrix multiplication using the dot product
  - Let $\mathbf{a}_j$ denote the jth column of $\mathbf{A}$

$$\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_r] \tag{5}$$

  - Replace the loop in (4) by a dot product

$$c_{ij} = \mathbf{a}_i^T \mathbf{b}_j, \qquad i = 1 : m, \qquad j = 1 : n \tag{6}$$

    * $\mathbf{a}_i^T$ is the ith column of $\mathbf{A}^T$ or the ith row of $\mathbf{A}$

```
function C = matmy(A, B)
% matmy: compute the matrix product C = AB using
% the dot product
   [m r] = size(A);
   [r n] = size(B);
      for i = 1:m
      for j = 1:n
         C(i,j) = dot(A(i,1:r)',B(1:r,j));
      end
   end
```

  - The range 1:r indicates an operation for an entire row or column
  - A ' denotes transposition
  - $A(i, 1 : r)$ is the ith row of $\mathbf{A}$

Matrix Multiplication with Saxpys

- Reorder the loop structure: regard the columns of $\mathbf{C}$ as linear combinations of those of $\mathbf{A}$

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix} = \begin{bmatrix} 5 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 7 \begin{bmatrix} 2 \\ 4 \end{bmatrix} & 6 \begin{bmatrix} 1 \\ 3 \end{bmatrix} + 8 \begin{bmatrix} 2 \\ 4 \end{bmatrix} \end{bmatrix}$$

  - compute $\mathbf{C} = \mathbf{AB}$ as

$$\mathbf{c}_j = \sum_{k=1}^{r} b_{kj} \mathbf{a}_k, \qquad j = 1 : n \tag{7}$$

  - Implement the sum using saxpys

```
function C = smatmy(A, B)
% smatmy: compute the matrix product C = AB
% using saxpys
   [m r] = size(A);
   [r n] = size(B);
   C = zeros(m, n);
   for j = 1:n
      for k = 1:r
         C(1:m,j) = saxpy(B(k,j), A(1:m,k), C(1:m,j));
      end
   end
```

  - zeros(m,n) returns a $m \times n$ matrix of zeros.

Outer Products

- Reorder the loops to perform an outer product
  - An *outer product* of an m-vector $\mathbf{x}$ and an n-vector $\mathbf{y}$ is the $m \times n$ matrix

$$\mathbf{C} = \mathbf{x}\mathbf{y}^T \tag{8}$$

    or

$$\mathbf{C} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} [y_1 y_2 \cdots y_n] = \begin{bmatrix} x_1y_1 & x_1y_2 & \cdots & x_1y_n \\ x_2y_1 & x_2y_2 & \cdots & x_2y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_my_1 & x_my_2 & \cdots & x_my_n \end{bmatrix}$$

  - *Problem 1*: do matrix multiplication using outer products
    - Show this for the 2×2 problem

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 5 & 6 \\ 7 & 8 \end{bmatrix}$$

Outer Product

$*$ Write an algorithm for a general system

- Different loop structures perform differently on different computers

dot product	i, j, k
saxpy	j, k, i
outer porduct	k, i, j

1.2. Special Matrices

- Complex Matrices
  - $\mathbf{A} \in C^{m \times n}$ implies that a_{ij} are complex numbers

$$a_{ij} = \alpha_{ij} + i\beta_{ij}, \qquad \alpha_{ij}, \beta_{ij} \in \Re,$$
$$i = 1, 2, ..., m, \qquad j = 1, 2, ..., n$$

  - Operations are the same except for:
    - Transposition: if $a_{ij} = \alpha_{ij} + i\beta_{ij}$ then

$$\mathbf{C} = \mathbf{A}^H = \bar{\mathbf{A}}^T, \qquad c_{ij} = \bar{a}_{ji} = \alpha_{ji} - i\beta_{ji}$$

    - Inner product: if $\mathbf{x}, \mathbf{y} \in C^n$ then

$$s = \mathbf{x}^H \mathbf{y} = \sum_{i=1}^{n} \bar{x}_i y_i$$

    - $\mathbf{x}^H \mathbf{x}$ is real

$$\mathbf{x}^H \mathbf{x} = \sum_{i=1}^{n} \bar{x}_i x_i = \sum_{i=1}^{n} |x_i|^2$$

Band Matrices

- **Definition 1**: $\mathbf{A} \in \Re^{m \times n}$ has *lower bandwidth* p if $a_{ij} = 0$ for $i > j + p$ and *upper bandwidth* q if $a_{ij} = 0$ for $j > i + q$.

$$\mathbf{A} = \begin{bmatrix} \times & \times & 0 & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & 0 \\ \times & \times & \times & \times & \times & 0 \\ 0 & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times \end{bmatrix}$$

  - The $\times$ denotes an arbitrary nonzero entry
  - This 8×6 matrix has lower bandwidth 3 and upper bandwidth 1
  - *Example 1.* A 5×7 upper triangular matrix $p = 0$, $q = 6$

$$\begin{bmatrix} \times & \times & \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times & \times & \times \\ 0 & 0 & \times & \times & \times & \times & \times \\ 0 & 0 & 0 & \times & \times & \times & \times \\ 0 & 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

Some Band Matrices

Matrix	p	q
Diagonal	0	0
Upper Triangular	0	$n-1$
Lower Triangular	$m-1$	0
Tridiagonal	1	1
Upper bidiagonal	0	1
Lower bidiagonal	1	0
Upper Hessenberg	1	$n-1$
Lower Hessenberg	$m-1$	1

- *Example 2.* A 5×6 tridiagonal matrix $p = q = 1$

$$\mathbf{A} = \begin{bmatrix} \times & \times & 0 & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 & 0 \\ 0 & \times & \times & \times & 0 & 0 \\ 0 & 0 & \times & \times & \times & 0 \\ 0 & 0 & 0 & \times & \times & \times \end{bmatrix}$$

- *Example 3.* A 4×6 Lower Hessenberg matrix $p = 3$, $q = 1$

$$\mathbf{A} = \begin{bmatrix} \times & \times & 0 & 0 & 0 & 0 \\ \times & \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & 0 & 0 \\ \times & \times & \times & \times & \times & 0 \end{bmatrix}$$

Lower by Upper Triangular Matrix Product

- *Example 4* (cf. Golub and Van Loan (1996), Problem 1.2.3, p. 23).
- $\mathbf{L}$ and $\mathbf{U}$ are $n \times n$ lower and upper triangular matrices
- Give a column saxpy algorithm for computing

$$\mathbf{C} = \mathbf{UL}$$

$$\begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix} \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} = [\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3]$$

- Express the columns of $\mathbf{C}$ as a linear combination of the columns of $\mathbf{U}$

$$\mathbf{c}_1 = \begin{bmatrix} u_{11} \\ 0 \\ 0 \end{bmatrix} l_{11} + \begin{bmatrix} u_{12} \\ u_{22} \\ 0 \end{bmatrix} l_{21} + \begin{bmatrix} u_{13} \\ u_{23} \\ u_{33} \end{bmatrix} l_{31}$$

$$\mathbf{c}_2 = \begin{bmatrix} u_{12} \\ u_{22} \\ 0 \end{bmatrix} l_{22} + \begin{bmatrix} u_{13} \\ u_{23} \\ u_{33} \end{bmatrix} l_{32}, \qquad \mathbf{c}_3 = \begin{bmatrix} u_{13} \\ u_{23} \\ u_{33} \end{bmatrix} l_{33}$$

Lower by Upper Triangular Matrix Product

- Use the saxpy matrix multiplication formula (1.7)

$$\mathbf{c}_j = \sum_{k=1}^{n} \mathbf{u}_k l_{kj}$$

- $l_{kj} = 0$ if $k < j$

$$\mathbf{c}_j = \sum_{k=j}^{n} \mathbf{u}_k l_{kj}$$

- $u_{ik} = 0$ if $i > k$

```
function C = suplow(U, L)
% suplow: compute the matrix product C = UL using saxpys
% where L and U are n × n lower and upper
% triangular matrices.
   [n n] = size(U);
   C = zeros(n);
   for j = 1:n
      for k = j:n
         C(1:k,j) = saxpy(L(k,j), U(1:k,k), C(1:k,j));
      end
   end
```

Lower by Upper Triangular Matrix Product

- Operation count:
  - A saxpy for a vector of length k requires k multiplications and k additions
  - The inner k loop has $n - j$ saxpys on vectors of length k and requires

$$\sum_{k=j}^{n} k$$

    multiplications and additions
    - Recall

$$\sum_{i=1}^{n} i = \frac{n(n+1)}{2} \tag{1}$$

    - The multiplications/additions in the inner loop are

$$\sum_{k=j}^{n} k = \sum_{k=1}^{n} k - \sum_{k=1}^{j-1} k = \frac{1}{2}[n(n+1) - (j-1)j]$$

  - The multiplications/additions in the outer loop are

$$\frac{1}{2}\sum_{j=1}^{n}[n(n+1) - (j-1)j]$$

    - Recall

$$\sum_{i=1}^{n} i^2 = \frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6} \tag{2}$$

Lower by Upper Triangular Matrix Product

- Thus, the total operation count is

$$\frac{1}{2}[n^2(n+1) - \frac{n^3}{3} - \frac{n^2}{2} - \frac{n}{6} + \frac{n(n+1)}{2}]$$

  or

$$\frac{1}{2}[\frac{2n^3}{3} + n^2 + \frac{n}{3}] = \frac{(n+1)(2n+1)n}{6}$$

  - For large n, there are approximately $n^3/3$ multiplications and additions

- Multiplication of two $n \times n$ full matrices requires n^3 multiplications and additions

Band-Matrix Storage

- Let $\mathbf{A} \in \Re^{n \times n}$ have lower and upper bandwidth p and q
  - If $p, q \ll n$ then store $\mathbf{A}$ in either a $(p+q+1) \times n$ or a $n \times (p+q+1)$ matrix $\mathbf{A}^{band}$ to save storage
  - *Example 5.* Consider a 8×8 matrix with $p = 3$ and $q = 1$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 & 0 & 0 & 0 \\ a_{31} & a_{32} & a_{33} & a_{34} & 0 & 0 & 0 & 0 \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} & 0 & 0 & 0 \\ 0 & a_{52} & a_{53} & a_{54} & a_{55} & a_{56} & 0 & 0 \\ 0 & 0 & a_{63} & a_{64} & a_{65} & a_{66} & a_{67} & 0 \\ 0 & 0 & 0 & a_{74} & a_{75} & a_{76} & a_{77} & a_{78} \\ 0 & 0 & 0 & 0 & a_{85} & a_{86} & a_{87} & a_{88} \end{bmatrix}$$

  - *Row Storage*: "slide" all rows to the left or right to align the columns on anti-diagonals

$$\mathbf{A}^{band} = \begin{bmatrix} 0 & 0 & 0 & a_{11} & a_{12} \\ 0 & 0 & a_{21} & a_{22} & a_{23} \\ 0 & a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} & a_{45} \\ a_{52} & a_{53} & a_{54} & a_{55} & a_{56} \\ a_{63} & a_{64} & a_{65} & a_{66} & a_{67} \\ a_{74} & a_{75} & a_{76} & a_{77} & a_{78} \\ a_{85} & a_{86} & a_{87} & a_{88} & 0 \end{bmatrix}$$

    - $\mathbf{A}^{band} \in \Re^{n \times p+q+1}$ with

$$a_{ij} = a^{band}_{i,j-i+p+1}$$

    - Can also store $\mathbf{A}$ by columns

Band Matrix-Vector Multiplication

- *Example 6.* Multiply a band matrix $\mathbf{A}$ by a vector $\mathbf{x}$

$$y_i = \sum_{j=\max(1,i-p)}^{\min(n,i+q)} a_{ij}x_j = \sum_{j=\max(1,i-p)}^{\min(n,i+q)} a^{band}_{i,j-i+p+1}x_j$$

function $\mathbf{y}$ = bmatvec(p, q, $\mathbf{A}^{band}$, $\mathbf{x}$)
% bmatvec: compute the matrix-vector product $\mathbf{y} = \mathbf{Ax}$
% where $\mathbf{A}^{band}$ is an $n \times n$ matrix stored in banded
% form by rows and $\mathbf{x}$ is an n-vector. The scalars p and q
% are the lower and upper bandwidths of $\mathbf{A}$, respectively.

% start and stop indicate the column index of the first and
% last nonzero entries in row i of $\mathbf{A}^{band}$.
% jstart and jstop indicate similar column indices for $\mathbf{A}$.

```
[n n] = size(A);
y(1:n) = 0;
for i = 1:n
   jstart = max(1, i-p);
   start = jstart - i + p + 1;
   jstop = min(n, i+q);
   stop = jstop - i + p + 1;
   y(i) = dot(A^band(i,start:stop)', x(jstart:jstop));
end
```

Symmetric Matrics

- **Definition 2**: $\mathbf{A} \in \Re^{n \times n}$ is *symmetric* if $\mathbf{A}^T = \mathbf{A}$

$$\mathbf{A} = \begin{bmatrix} 13 & 9 & -1 \\ 9 & 4 & 7 \\ -1 & 7 & -8 \end{bmatrix}$$

  - Only half of the matrix need be stored
  - Store the lower or upper triangular part of $\mathbf{A}$ as a vector

$$\mathbf{a}^{sym} = [13, 9, -1, 4, 7, -8]$$

  - Store the upper triangular part of $\mathbf{A}$ by rows

$$a_{ij} = a^{sym}_{(i-1)n - i(i-1)/2 + j} \tag{3a}$$

  - Arrange storage so that inner loops access contiguous data
    - *FORTRAN* stores matrices by columns
    - *C* stores matrices by rows
  - Symmetric matrix by vector multiplication

$$y_i = \sum_{j=1}^{n} a_{ij} x_j = \sum_{j=1}^{i-1} a_{ji} x_j + \sum_{j=i}^{n} a_{ij} x_j \tag{3b}$$

- Can also store $\mathbf{A}$ by diagonals

Block Matrices

- Partition the rows and columns of $\mathbf{A} \in \Re^{m \times n}$ into submatrices such that

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \cdots & \mathbf{A}_{1q} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \cdots & \mathbf{A}_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}_{p1} & \mathbf{A}_{p2} & \cdots & \mathbf{A}_{pq} \end{bmatrix}$$

  - $\mathbf{A}_{ij} \in R^{m_i \times n_j}$, $i = 1 : m$, $j = 1 : n$
  - $m_1 + m_2 + ... + m_p = m$, $n_1 + n_2 + ... + n_q = n$
  - All operations on matrices with scalar components apply to those with matrix components
    - Matrix operations on the blocks are required
  - Let $\mathbf{B} \in \Re^{k \times l}$

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} & \cdots & \mathbf{B}_{1s} \\ \mathbf{B}_{21} & \mathbf{B}_{22} & \cdots & \mathbf{B}_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{B}_{r1} & \mathbf{B}_{r2} & \cdots & \mathbf{B}_{rs} \end{bmatrix}$$

    - $\mathbf{B}_{ij} \in \Re^{k_i \times l_j}$, $i = 1 : k$, $j = 1 : l$
    - $k_1 + k_2 + ... + k_r = k$, $l_1 + l_2 + ... + l_s = l$

Block Matrix Addition and Multiplication

- *Addition*: a partition is *conformable* for addition if
  - $m = k$, $n = l$, $p = r$, $q = s$
  - $m_i = k_i$, $n_j = l_j$, $i = 1 : m$, $j = 1 : l$
  - Then $\mathbf{C} = \mathbf{A} + \mathbf{B}$ with $\mathbf{C}_{ij} = \mathbf{A}_{ij} + \mathbf{B}_{\mathbf{ij}}$, $i = 1 : p$, $j = 1 : q$

- *Multiplication*: a partition is *conformable* for multiplication if
  - $n = k$, $q = r$, $n_j = k_j$, $j = 1 : q$
  - Then

$$\mathbf{C} = \mathbf{AB} = \begin{bmatrix} \mathbf{C}_{11} & \mathbf{C}_{12} & \cdots & \mathbf{C}_{1s} \\ \mathbf{C}_{21} & \mathbf{C}_{22} & \cdots & \mathbf{C}_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{C}_{p1} & \mathbf{C}_{p2} & \cdots & \mathbf{C}_{ps} \end{bmatrix} \tag{4a}$$

with

$$\mathbf{C}_{ij} = \sum_{t=1}^{q} \mathbf{A}_{it}\mathbf{B}_{tj}, \qquad i = 1 : p, \qquad j = 1 : s \tag{4b}$$

Sparse Matrices

- *Definition*
  - Sparse matrices have a "significant" number of zeros
  - A matrix is considered to be sparse if the zeros are neither to be stored nor operated upon
- *Motivation*
  - Sparse matrices with arbitrary zero structures arise in finite element and network problems

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 2 & 0 \\ 3 & 4 & 0 & 5 & 0 \\ 6 & 0 & 7 & 8 & 9 \\ 0 & 0 & 10 & 11 & 0 \\ 0 & 0 & 0 & 0 & 12 \end{bmatrix}$$

- *Storage*
  - Store $\mathbf{A}$ as a vector $\mathbf{a}$ by rows or columns
  - An integer vector $\mathbf{ja}$ stores the column indices of $\mathbf{A}$
    - when $\mathbf{A}$ is stored by rows
  - A second vector $\mathbf{ia}$ stores the indices in $\mathbf{ja}$ of the first element of each row of $\mathbf{A}$
    - The last element of $\mathbf{ia}$, $ia_n + 1$, usually signals termination

Sparse Matrices

- For example

$$\mathbf{a} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \end{bmatrix} \qquad \mathbf{ja} = \begin{bmatrix} 1 \\ 4 \\ 1 \\ 2 \\ 4 \\ 1 \\ 3 \\ 4 \\ 5 \\ 3 \\ 4 \\ 5 \end{bmatrix} \qquad \mathbf{ia} = \begin{bmatrix} 1 \\ 3 \\ 6 \\ 10 \\ 12 \\ 13 \end{bmatrix}$$

- The dimension of **a** and **ja** is the number of nonzeros in **A**. That of **ia** is $n + 1$
  - $ia_n + 1$ is set to the beginning index of a ficticious row $n + 1$
- The storage scheme is called the *compressed sparse row (CSR)* format
  - CSC is the *compressed sparse column* format
- Linked structures can be used instead of arrays

Sparse Matrices

- *Example 7.* Multiply a sparse matrix **A** by a vector **x**

```
function y = smatvec(a, ja, ia, x)
% smatvec: compute the matrix-vector product y = Ax
% where a is the n-by-n matrix A stored in CSR
% format, ja is a vector of pointers to the nonzero elements
% of A, ia is a vector pointing to the first nonzero
% element in each row of A.

   n = length(ia) - 1;
   for i = 1:n

% start and stop locate the beginning
% and end of row i in a and ja.

   start = ia(i);
   stop = ia(i+1) - 1;
   y(i) = 0;
   for k = start:stop
      y(i) = y(i) + a(k)*x(ja(k));
   end
end
```

- cf. Y. Saad (1996), *Iterative Methods for Sparse Linear Systems,* PWS, Boston, Section 3.4.

2. Gaussian Elimination

2.1. Vector and Matrix Norms

- *(Linear) Vector Space*. Regard the columns (rows) of a matrix $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ as forming a vector space $\Re^{m \times n}$
  - The key properties of a vector space $\mathcal{V}$ are
    i. If $\mathbf{u}, \mathbf{v} \in V$ then $\mathbf{u} + \mathbf{v} \in \mathcal{V}$
    ii. If $\mathbf{u} \in V$ and $\alpha \in \Re$ then $\alpha \mathbf{u} \in \mathcal{V}$
  - The definition appears in, e.g., K. Hoffman and R. Kunze (1971), *Linear algebra*, Second Edition, Prentice Hall, Englewood Cliffs
  - A *subspace* of $\mathcal{V}$ is a subset that is also a vector space
- **Definition 1**: A set of vectors $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\} \in \Re^{m \times n}$ is *linearly independent* if the only solution of

$$\sum_{j=1}^{n} \alpha_j \mathbf{a}_j = 0$$

is $\alpha_j = 0$, $j = 1 : n$

Subspaces

- **Definition 2**: The set of all linear combinations of

$$\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\} \in \Re^{m \times n}$$

  is a vector space called the *linear span* of $\Re^{m \times n}$:

$$\text{span}(\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}) = \left\{ \sum_{j=1}^{n} \alpha_j \mathbf{a}_j | \alpha_j \in \Re \right\} \qquad (1)$$

  - **Theorem 1**: If $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ is linearly independent then $\mathbf{u} \in \text{span}(\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\})$ is unique

- **Definition 3**: Let $\mathcal{S}_1, \mathcal{S}_2 \subset \Re^{m \times n}$, then

  i. Their *sum* is the subspace $\{\mathbf{a}_1 + \mathbf{a}_2 | \mathbf{a}_1 \in \mathcal{S}_1, \mathbf{a}_2 \in \mathcal{S}_2\}$

  ii. If $\mathcal{S}_1 \cap \mathcal{S}_2$ is $\emptyset$ then the sum of $\mathcal{S}_1$ and $\mathcal{S}_2$ is called the *direct sum* and is written as $\mathcal{S}_1 \oplus \mathcal{S}_2$

- **Definition 4**: A subset $\mathcal{S}$ is a *maximal linearly independent subset* of $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ if:

  i. it is linearly independent

  ii. it is not properly contained in any linearly independent subset of $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$

- **Definition 5**: A maximal linearly independent set $\{\mathbf{b}_1, \mathbf{b}_2, ..., \mathbf{b}_k\}$ forms a *basis* for $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$

Range, Null Space, and Rank

- Some properties:
  i. If $\{\mathbf{b}_1, \mathbf{b}_2, ..., \mathbf{b}_k\}$ is a basis for $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ then
  $$\text{span}(\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}) = \text{span}(\{\mathbf{b}_1, \mathbf{b}_2, ..., \mathbf{b}_k\})$$
  ii. All bases for $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ have the same number of elements
  iii. This number is the *dimension* of $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\}$ and is written as $\dim(\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\})$
- **Definition 6**: If $\mathbf{A} \in \Re^{m \times n}$ then:
  i. The *range* of $\mathbf{A}$ satisfies
  $$\text{range}(\mathbf{A}) = \{\mathbf{y} \in \Re^m | \mathbf{y} = \mathbf{A}\mathbf{x}, \mathbf{x} \in \Re^n\} \quad (2)$$
  ii. The *null space* of $\mathbf{A}$ satisfies
  $$\text{null}(\mathbf{A}) = \{\mathbf{x} \in \Re^n | \mathbf{A}\mathbf{x} = 0\} \quad (3)$$
- For $\mathbf{A} \in \Re^{m \times n}$
  i. $\text{range}(\mathbf{A}) = \text{span}(\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_n\})$
  ii. The *rank* of $\mathbf{A}$ satisfies $\text{rank}(\mathbf{A}) = \dim(\text{range}(\mathbf{A}))$
  iii. $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}^T)$
    – $\text{rank}(\mathbf{A})$ is the number of independent rows or columns of $\mathbf{A}$
  iv. $\dim(\text{null}(\mathbf{A})) + \text{rank}(\mathbf{A})) = n$

Inverses

- The $n \times n$ identity matrix is

$$\mathbf{I} = [\mathbf{e}_1, \mathbf{e}_2, ..., \mathbf{e}_n] = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots \\ 0 & 0 & \cdots & 1 \end{bmatrix} \tag{4}$$

- If $\mathbf{A}, \mathbf{X} \in \Re^{n \times n}$ and

$$\mathbf{AX} = \mathbf{I}$$

  then $\mathbf{X}$ is called the *inverse of* $\mathbf{A}$ and is written as $\mathbf{A}^{-1}$

  - If $\mathbf{A}^{-1}$ does not exist then $\mathbf{A}$ is called *singular*, otherwise *nonsingular*.
  - Some properties:

$$(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1} \tag{5a}$$

$$(\mathbf{A}^{-1})^T = (\mathbf{A}^T)^{-1} := \mathbf{A}^{-T} \tag{5b}$$

Determinants

- The *determinant* of a matrix $\mathbf{A} \in \Re^{n \times n}$ satisfies

$$\det(\mathbf{A}) = \begin{cases} a_{11}, & \text{if } n = 1 \\ \sum_{j=1}^{n} (-1)^{j+1} a_{1j} \det(\mathbf{A_{1j}}), & \text{if } n > 1 \end{cases} \tag{6}$$

  where $\mathbf{A}_{1j}$ is an $(n-1) \times (n-1)$ matrix obtained by deleting the first row and column of $\mathbf{A}$

  - The definition is recursive
  - Some properties:

$$\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B}) \tag{7a}$$

$$\det(\mathbf{A}^T) = \det(\mathbf{A}) \tag{7b}$$

$$\det(\alpha \mathbf{A}) = \alpha^n \det(\mathbf{A}), \qquad \alpha \in \Re \tag{7c}$$

    * $\det(\mathbf{A}) \neq 0$ if and only if $\mathbf{A}$ is nonsingular

Vector Norms

- Reading: Trefethen and Bau (1997), Lecture 3
- Norms provide a way to measure distances between vectors and matrices
  - They provide a measure of "closeness" that is used to understand convergence
- **Definition 7**: A *vector norm* $||\cdot||$ is a functional ($||\cdot|| : \Re^n \rightarrow \Re$) satisfying
  - i. $||\mathbf{x}|| \geq 0, \qquad ||\mathbf{x}|| = 0 \leftrightarrow \mathbf{x} = 0, \mathbf{x} \in \Re^n$
  - ii. $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||, \mathbf{x}, \mathbf{y} \in \Re^n$
  - iii. $||\alpha\mathbf{x}|| = |\alpha|||\mathbf{x}||, \alpha \in \Re, \mathbf{x}, \mathbf{y} \in \Re^n$
- The p-norms are the most useful to us:

$$||\mathbf{x}||_p = (|x_1|^p + |x_2|^p + ... + |x_n|^p)^{1/p}, \qquad p \geq 1 \tag{8}$$

  - The most important of these are

$$||\mathbf{x}||_1 = |x_1| + |x_2| + ... + |x_n| \tag{9a}$$

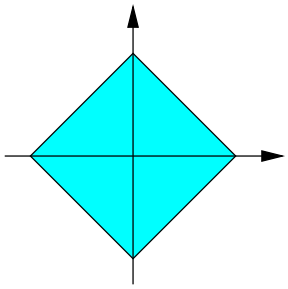
$$||\mathbf{x}||_2 = (|x_1|^2 + |x_2|^2 + ... + |x_n|^2)^{1/2} \tag{9b}$$

$$||\mathbf{x}||_\infty = \max_{1 \leq i \leq n} |x_i| \tag{9c}$$

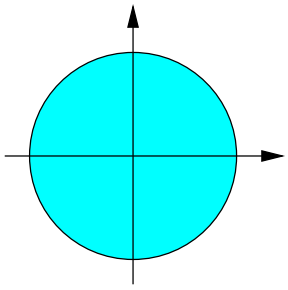
Vector Norms

- For $\mathbf{x} \in \Re^2$

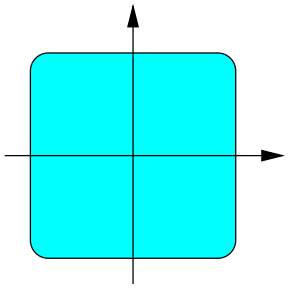
$||\mathbf{x}||_1 = |x_1| + |x_2|$



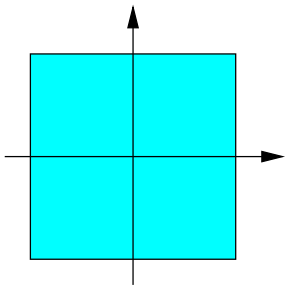
$||\mathbf{x}||_2 = (|x_1|^2 + |x_2|^2)^{1/2}$



$||\mathbf{x}||_p = (|x_1|^p + |x_2|^p)^{1/p}, 1 < p < \infty$



$||\mathbf{x}||_\infty = \max(|x_1|, |x_2|)$



Vector Norms

- Some properties of p-norms
  - The *Holder inequality:*

$$|\mathbf{x}^T\mathbf{y}| \leq ||\mathbf{x}||_p||\mathbf{y}||_q, \qquad \frac{1}{p}+\frac{1}{q}=1 \tag{10a}$$

  - The *Cauchy-Schwartz inequality* $(p = q = 2)$

$$|\mathbf{x}^T\mathbf{y}| \leq ||\mathbf{x}||_2||\mathbf{y}||_2 \tag{10b}$$

  - **Theorem 2**: p-norms are equivalent in the sense that there exist constants $c, C > 0$ such that

$$c||\mathbf{x}||_\alpha \leq ||\mathbf{x}||_\beta \leq C||\mathbf{x}||_\alpha \tag{11}$$

    * For example

$$||\mathbf{x}||_\infty \leq ||\mathbf{x}||_1 \leq n||\mathbf{x}||_\infty \tag{12a}$$

$$||\mathbf{x}||_\infty \leq ||\mathbf{x}||_2 \leq \sqrt{n}||\mathbf{x}||_\infty \tag{12b}$$

$$||\mathbf{x}||_2 \leq ||\mathbf{x}||_1 \leq \sqrt{n}||\mathbf{x}||_2 \tag{12c}$$

Vector Norms

- *Example 1* (cf. Trefethen and Bau (1997)), Problem 3.3). Verify (12)

Matrix Norms

- Matrix norms measure the sensitivity of a matrix to perturbations
- The definition of a matrix norm is identical to that of a vector norm
- **Definition 8**: A *matrix norm* $||\mathbf{A}||$, $\mathbf{A} \in \Re^{m \times n}$, is a functional satisfying

  i. $||\mathbf{A}|| \geq 0, \qquad ||\mathbf{A}|| = 0 \leftrightarrow \mathbf{A} = 0$

  ii. $||\mathbf{A} + \mathbf{B}|| \leq ||\mathbf{A}|| + ||\mathbf{B}||$

  iii. $||\alpha \mathbf{A}|| = |\alpha| ||\mathbf{A}||, \alpha \in \Re$

- Vector induced matrix norms are defined in terms of p-norms of vectors

$$||\mathbf{A}||_p = \max_{\mathbf{x} \neq 0} \frac{||\mathbf{A}\mathbf{x}||_p}{||\mathbf{x}||_p} \tag{13a}$$

  – Letting $\mathbf{y} = \mathbf{x}/||\mathbf{x}||_p$, yields the equivalent definition

$$||\mathbf{A}||_p = \max_{||\mathbf{x}||=1} ||\mathbf{A}\mathbf{x}||_p \tag{13b}$$

  – There are also pq-norms

$$||\mathbf{A}||_{pq} = \max_{\mathbf{x} \neq 0} \frac{||\mathbf{A}\mathbf{x}||_p}{||\mathbf{x}||_q} \tag{13c}$$

Matrix Norms

- Properties of matrix norms:
  - From (13a), it is clear that

$$||\mathbf{Ax}||_p \leq ||\mathbf{A}||_p ||\mathbf{x}||_p \tag{14a}$$

    and, more generally,

$$||\mathbf{AB}||_p \leq ||\mathbf{A}||_p ||\mathbf{B}||_p, \qquad \mathbf{A} \in \Re^{m \times n}, \qquad \mathbf{B} \in \Re^{n \times r} \tag{14b}$$

    * Matrix norms that satisfy (14b) are called *consistent.*
  - As a further consequence of (14b)

$$||\mathbf{A}^k||_p \leq ||\mathbf{A}||_p^k$$

- Matrix p norms corresponding to vector p-norms are

$$||\mathbf{A}||_1 = \max_{1 \leq j \leq n} \sum_{i=1}^{m} |a_{ij}| \tag{15a}$$

$$||\mathbf{A}||_\infty = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |a_{ij}| \tag{15b}$$

$$||\mathbf{A}||_2 = [\rho(\mathbf{A}^T \mathbf{A})]^{1/2} \tag{15c}$$

  - The *spectral radius* $\rho(\mathbf{A})$ is the magnitude of the largest eigenvalue of a matrix $\mathbf{A} \in \Re^{n \times n}$.

Frobenius Matrix Norm

- p norms
  - The 1-norm is the maximum absolute column sum
  - The ∞-norm is the maximum absolute row sum
  - The 2-norm requires an eigenvalue analysis
- The *Frobenius norm*:

$$||\mathbf{A}||_F = \left[\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \right]^{1/2} \tag{16a}$$

  - It is not a p-norm
  - It can be viewed as the 2-norm of a vector in $\Re^{mn}$
  - It satisfies (14b)
  - It has the equivalent definition

$$||\mathbf{A}||_F = [\mathrm{tr}(\mathbf{A}^T\mathbf{A})]^{1/2} = [\mathrm{tr}(\mathbf{A}\mathbf{A}^T)]^{1/2} \tag{16b}$$

    where

$$\mathrm{tr}(\mathbf{A}) = \sum_{i=1}^{n} a_{ii}, \qquad \mathbf{A} \in \Re^{n \times n} \tag{16c}$$

Fun with Norms

- *Example 2.* Calculate the 1, 2, ∞, and F norms of

$$\mathbf{A} = \begin{bmatrix} 1 & -3 & 6 \\ 4 & 7 & -3 \\ -2 & 5 & 9 \\ 3 & -2 & 4 \end{bmatrix}$$

  - The column sums are

$$\sum_{i=1}^{4} |a_{i1}| = \quad , \quad \sum_{i=1}^{4} |a_{i2}| = \quad , \quad \sum_{i=1}^{4} |a_{i3}| =$$

    Thus,

$$||\mathbf{A}||_1 =$$

  - The row sums are

$$\sum_{j=1}^{3} |a_{1j}| = \quad , \quad \sum_{j=1}^{3} |a_{2j}| =$$

$$\sum_{j=1}^{3} |a_{3j}| = \quad , \quad \sum_{j=1}^{3} |a_{4j}| =$$

    Thus,

$$||\mathbf{A}||_\infty =$$

More Fun

- The product of $\mathbf{A}$ and $\mathbf{A}^T$ is

$$\mathbf{A}^T\mathbf{A} = \begin{bmatrix} 30 & 9 & -12 \\ 9 & 87 & -2 \\ -12 & -2 & 142 \end{bmatrix}$$

- The eigenvalues of $\mathbf{A}^T\mathbf{A}$ are 88.1293, 27.4447, and 143.4260
- Thus,

$$||\mathbf{A}||_2 = \sqrt{143.4260} = 11.9761$$

- Also $||\mathbf{A}||_F = 16.0935$
- **Theorem 3**: If $\mathbf{A} \in \Re^{m\times n}$ then

$$||\mathbf{A}||_2^2 \leq ||\mathbf{A}||_1||\mathbf{A}||_\infty \tag{17}$$

  - *Proof*: $\mu = ||\mathbf{A}||_2$ satisfies

$$\mathbf{A}^T\mathbf{A}\mathbf{z} = \mu^2\mathbf{z}$$

    μ^2 is the largest eigenvalue of $\mathbf{A}^T\mathbf{A}$ and $\mathbf{z}$ is the corresponding eigenvector

  - Take the 1 norm and use (14b) and (15a,b)

$$\begin{aligned} \mu^2||\mathbf{z}||_1 = ||\mathbf{A}^T\mathbf{A}\mathbf{z}||_1 &\leq ||\mathbf{A}^T||_1||\mathbf{A}||_1||\mathbf{z}||_1 \\ &= ||\mathbf{A}||_\infty||\mathbf{A}||_1||\mathbf{z}||_1 \end{aligned}$$

  - Divide by $||\mathbf{z}||_1$

- For Example 2, $||\mathbf{A}||_2 \leq \sqrt{(22)(16)} = 18.7617$

Spectral Radii and Norms

- **Theorem 4**: For $\mathbf{A} \in \Re^{n \times n}$

$$\rho(\mathbf{A}) \leq ||\mathbf{A}||_p \tag{18}$$

  - Let λ be the eigenvalue of $\mathbf{A}$ corresponding to the spectral radius and $\mathbf{z}$ be the corresponding eigenvector
    - $\rho(\mathbf{A}) = |\lambda|$
  - Consider

$$\mathbf{A}\mathbf{z} = \lambda\mathbf{z}$$

  - Take a p norm

$$||\mathbf{A}\mathbf{z}||_p = \rho(\mathbf{A})||\mathbf{z}||_p$$

    or

$$\rho(\mathbf{A}) = \frac{||\mathbf{A}\mathbf{z}||_p}{||\mathbf{z}||_p} \leq \max_{x \neq 0} \frac{||\mathbf{A}\mathbf{x}||_p}{||\mathbf{x}||_p} = ||\mathbf{A}||_p$$

2.2. Finite Precision Arithmetic

- Reading: Trefethen and Bau (1997), Lectures 12-15
- Real numbers are approximated by floating point numbers
- *Real number:*

$$x = \pm d_0.d_1 d_2 \cdots d_{t-1} d_t \cdots \times \beta^e \tag{1a}$$

  β The base of the number system
  d_i β-digits, $0 \le d_i < \beta$
  $d_0 \neq 0$ unless $x = 0$
  e Exponent

- *Floating point number:*

$$x \approx fl(x) = \pm d_0.d_1 d_2 \cdots d_{t-1} \times \beta^e \tag{1b}$$

  t Precision
  e $m \le e \le M$

  – Approximate x by
    Chopping: Set $d_t = d_{t+1} = \cdots = 0$
    Rounding: Add $\mathrm{sgn}(x)\beta/2 \times \beta^{e-t}$ to x and chop
  – The approximation satisfies

$$fl(x) = x(1+\epsilon), \qquad |\epsilon| \le u \tag{2a}$$

  – where u is the *unit roundoff error*

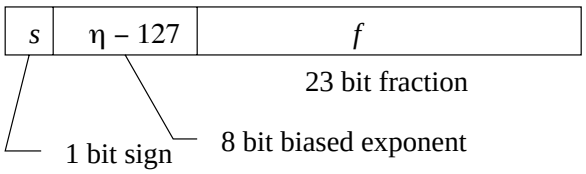
$$u = \begin{cases} \beta^{1-t}, & \text{with chopping} \\ \beta^{1-t}/2, & \text{with rounding} \end{cases} \tag{2b}$$

  – The *relative error* is

$$\frac{|fl(x) - x|}{|x|} \le u \tag{2c}$$

Floating Point Standards

- IEEE binary ($\beta = 2$) single-precision standard



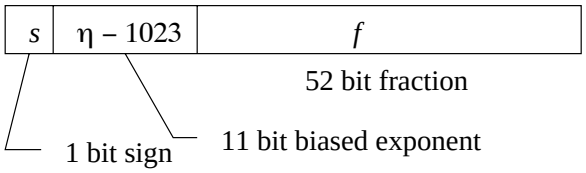
  - Represented number: $(-1)^s 2^{\eta-127}(1+f)$
    - s Sign (0 positive, 1 negative)
    - η Displaced exponent
    - f Fraction: bits $d_1 : d_t$ (d_0 is set to 1 and not stored)

Decimal	s	Exponent	Fraction
$+0$	0	00000000	00000000000000000000000
-0	1	00000000	00000000000000000000000
$+1$	0	01111111	00000000000000000000000
-1	1	01111111	00000000000000000000000
2^{-126}	0	00000001	00000000000000000000000
$2^{127}(2-2^{-23})$	0	11111110	11111111111111111111111
$+\infty$	0	11111111	00000000000000000000000
$-\infty$	1	11111111	00000000000000000000000
NaN	?	11111111	Anything but all zeros
Denormal	?	00000000	Anything but all zeros

  - *Underflow threshold*: $2^{-126} \approx 1.17 \times 10^{-38}$
  - *Overflow threshold*: $2^{127}(2-2^{-23}) \approx 2^{128} \approx 3.40 \times 10^{38}$
  - *NaN*: not a number
  - *Denormal*: un-normalized number ($d_0 = 0$)
  - $u = 2^{-24} \approx 5.96 \times 10^{-8}$

Floating Point Standards

- IEEE binary double-precision standard



  - Represented number: $(-1)^s 2^{\eta-1023}(1+f)$
  - *Underflow threshold*: $2^{-1022} \approx 2.23 \times 10^{-308}$
  - *Overflow threshold*: $2^{1023}(2-2^{-52}) \approx 2^{1024} \approx 1.80 \times 10^{308}$
  - $u = 2^{-53} \approx 1.11 \times 10^{-16}$

Stability

- Assume that an operation $\odot$ $(+, -, *, /, \sqrt{\ })$ satisfies

$$fl(a \odot b) = a \odot b(1 + \epsilon), \qquad |\epsilon| \leq u \tag{3a}$$

  - The *relative error* is

$$\frac{|fl(a \odot b) - a \odot b|}{|a \odot b|} \leq u \tag{3b}$$

- Analyze the roundoff error in computing a dot product

```
s = 0;
for k = 1:n
   s = s + x(k)*y(k);
end
```

- Let

$$s_p = fl\left(\sum_{k=1}^{p} x_k y_k\right)$$

- From the algorithm

$$s_p = (s_{p-1} + x_p y_p(1 + \delta_p))(1 + \epsilon_p), \qquad |\epsilon_j|, |\delta_j| \leq u$$

- With $p = 1$

$$s_1 = x_1 y_1(1 + \delta_1), \qquad |\delta_1| \leq u$$

  - Write this as

$$s_1 = x_1 y_1(1 + \delta_1)(1 + \epsilon_1), \qquad \epsilon_1 = 0$$

- With $p = 2$

$$s_2 = (s_1 + x_2 y_2(1 + \delta_2))(1 + \epsilon_2)$$

or

$$s_2 = x_1 y_1(1 + \delta_1)(1 + \epsilon_1)(1 + \epsilon_2) + x_2 y_2(1 + \delta_2)(1 + \epsilon_2)$$

Roundoff Error in a Dot Product

- With $p = 3$

$$s_3 = x_1y_1(1+\delta_1)(1+\epsilon_1)(1+\epsilon_2)(1+\epsilon_3)$$
$$+x_2y_2(1+\delta_2)(1+\epsilon_2)(1+\epsilon_3)$$
$$+x_3y_3(1+\delta_3)(1+\epsilon_3)$$

- With $p = n$

$$fl(\mathbf{x}^T\mathbf{y}) = s_n = \sum_{k=1}^{n} x_k y_k(1+\gamma_k) \tag{4a}$$

  where

$$1+\gamma_k = (1+\delta_k)\prod_{j=k}^{n}(1+\epsilon_j) \tag{4b}$$

- Expand (4b)

$$1+\gamma_k = 1+\delta_k+\sum_{j=k}^{n}\epsilon_j + O(u^2)$$

- Since $|\epsilon_j|$, $|\delta_j| \leq u$, $j = 1:n$

$$|\gamma_k| \leq (n-k+1)u + O(u^2)$$

  – Set $k = 1$ for simplicity

$$|\gamma_k| \leq nu + O(u^2)$$

Roundoff Error in a Dot Product

- Use (4a)

$$|fl(\mathbf{x}^T\mathbf{y}) - \mathbf{x}^T\mathbf{y}| \leq \sum_{k=1}^{n} |x_k y_k|(nu + O(u^2))$$

  - Let $|\mathbf{y}|$ be a vector with elements $|y_k|$, $k = 1:n$
  - Write

$$\sum_{k=1}^{n} |x_k y_k| := |\mathbf{x}|^T|\mathbf{y}|$$

- Then

$$|fl(\mathbf{x}^T\mathbf{y}) - \mathbf{x}^T\mathbf{y}| \leq nu|\mathbf{x}|^T|\mathbf{y}| + O(u^2)$$

- Dotting the is and crossing the ts

  - There is a $C \approx 1$

$$\begin{aligned} nu|\mathbf{x}|^T|\mathbf{y}| + O(u^2) &= nu|\mathbf{x}|^T|\mathbf{y}|(1 + O(u)) \\ &\leq Cnu|\mathbf{x}|^T|\mathbf{y}| \end{aligned}$$

  - Golub and van Loan (1996): $C = 1.01$ if $nu < 0.01$

- We have

$$\frac{|fl(\mathbf{x}^T\mathbf{y}) - \mathbf{x}^T\mathbf{y}|}{|\mathbf{x}^T\mathbf{y}|} \leq Cnu\frac{|\mathbf{x}|^T|\mathbf{y}|}{|\mathbf{x}^T\mathbf{y}|} \tag{5}$$

  - The relative error may not be small since $|\mathbf{x}^T\mathbf{y}|$ can be much less than $|\mathbf{x}|^T|\mathbf{y}|$

Backward Error Analysis

- Prior analysis is called *forward error analysis*
  - Relate rounding errors to the solution
- *Backward error analysis:*
  - Relate rounding errors to the original data
- Consider the dot-product computation
  - Write (4a) as

$$fl(\mathbf{x}^T\mathbf{y}) = \hat{\mathbf{x}}^T\hat{\mathbf{y}} \tag{6a}$$

    * $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ are perturbed values of $\mathbf{x}$, $\mathbf{y}$
    * The rounded dot product $fl(\mathbf{x}^T\mathbf{y})$ is the exact dot product $\hat{\mathbf{x}}^T\hat{\mathbf{y}}$ of perturbed vectors
  - Using (4a)

$$\hat{\mathbf{x}} = \begin{bmatrix} x_1\sqrt{1+\gamma_1} \\ x_2\sqrt{1+\gamma_2} \\ \vdots \\ x_n\sqrt{1+\gamma_n} \end{bmatrix}, \qquad \hat{\mathbf{y}} = \begin{bmatrix} y_1\sqrt{1+\gamma_1} \\ y_2\sqrt{1+\gamma_2} \\ \vdots \\ y_n\sqrt{1+\gamma_n} \end{bmatrix} \tag{6b}$$

  - Let $\boldsymbol{\delta x}$, $\boldsymbol{\delta y}$ be perturbations, i.e.,

$$\hat{\mathbf{x}} = \mathbf{x} + \boldsymbol{\delta x}, \qquad \hat{\mathbf{y}} = \mathbf{y} + \boldsymbol{\delta y}$$

Backward Error Analysis

- Observe that

$$\sqrt{1+\gamma_k} = 1 + \gamma_k/2 + O(\gamma_k^2)$$

- Thus,

$$\boldsymbol{\delta x} = \begin{bmatrix} x_1(\gamma_1/2 + O(\gamma_1^2)) \\ x_2(\gamma_2/2 + O(\gamma_2^2)) \\ \vdots \\ x_n(\gamma_n/2 + O(\gamma_n^2)) \end{bmatrix}$$

- But $|\gamma_k| \leq nu + O(u^2)$, so

$$|\boldsymbol{\delta x}| \leq \frac{nu}{2}|\mathbf{x}| + O(u^2) \tag{7a}$$

and

$$|\boldsymbol{\delta y}| \leq \frac{nu}{2}|\mathbf{y}| + O(u^2) \tag{7b}$$

- These bounds are very conservative

2.3. Factorizations

- Reading: Trefethen and Bau (1997), Lecture 20
- Solve the $n \times n$ linear system

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1}$$

  by Gaussian elimination
  - Gaussian elimination is a direct method
    - The solution is found after a finite number of operations
  - Iterative methods find a solution as the number of operations tend to infinity
    - Iteration is superior for large sparse systems
- Gaussian elimination is a factorization of $\mathbf{A}$ as

$$\mathbf{A} = \mathbf{L}\mathbf{U} \tag{2a}$$

  - $\mathbf{L}$ is unit lower triangular and $\mathbf{U}$ is upper triangular

LU Factorization

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \tag{2b}$$

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ l_{21} & 1 & \cdots & 0 \\ l_{31} & l_{32} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \cdots & 1 \end{bmatrix}, \qquad \mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ & 0 & & u_{3n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix} \tag{2c}$$

- Once $\mathbf{L}$ and $\mathbf{U}$ have been determined

$$\mathbf{Ax} = \mathbf{LUx} = \mathbf{b}$$

  - Let

$$\mathbf{Ux} = \mathbf{y} \tag{3a}$$

  - Then

$$\mathbf{Ly} = \mathbf{b} \tag{3b}$$

  - Solve (3b) for $\mathbf{y}$ by forward substitution and (3a) for $\mathbf{x}$ by backward substitution

LU Factorization

- *Classical Gaussian elimination*
  - Use row saxpys to reduce $\mathbf{A}$ to upper triangular form $\mathbf{U}$
  - Show that these row operations are the product of $\mathbf{A}$ and lower triangular matrices $\mathbf{L}_k$, $k = 1 : n-1$, i.e.,

$$\mathbf{L}_{n-1} \cdots \mathbf{L}_2 \mathbf{L}_1 \mathbf{A} = \mathbf{U} \tag{4a}$$

  - Thus

$$\mathbf{L} = \mathbf{L}_1^{-1} \mathbf{L}_2^{-1} \cdots \mathbf{L}_{n-1}^{-1} \tag{4b}$$

  - cf. Trefethen and Bau (1997), Lecture 20

- We use a direct factorization
  - Multiply the first row of $\mathbf{L}$ by $\mathbf{U}$ to obtain the first row of $\mathbf{A}$

$$a_{1j} = (1)u_{1j}, \qquad j = 1 : n$$

    * Thus

$$u_{1j} = a_{1j}, \qquad j = 1 : n$$

  - Multiply $\mathbf{L}$ by the first column of $\mathbf{U}$ to obtain the first column of $\mathbf{A}$

$$l_{i1} u_{11} = a_{i1}, \qquad i = 2 : n$$

    or

$$l_{i1} = a_{i1}/u_{11}, \qquad i = 2 : n$$

    * Redundant information with $i = 1$ is not written
    * The algorithm fails if $u_{11} = a_{11} = 0$

LU Factorization

- Continuing
  - Multiply the second row of **L** by **U** to obtain the second row of **A**

$$l_{21}u_{1j} + u_{2j} = a_{2j}, \qquad j = 2 : n$$

    * Thus,

$$u_{2j} = a_{2j} - l_{21}u_{1j}, \qquad j = 2 : n$$

  - The general procedure is

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj}, \qquad j = i : n, \tag{5a}$$

$$l_{ji} = \frac{1}{u_{ii}}(a_{ji} - \sum_{k=1}^{i-1} l_{jk}u_{ki}), \qquad j = i+1 : n, \quad i = 1 : n-1 \tag{5b}$$

    * The sums are zero when the lower limit exceeds the upper one
    * The procedure fails if $u_{ii} = 0$ for some i
    * The matrices **L** and **U** can be stored in the locations used for the same elements of **A**

LU Factorization

```
function A = lufactor(A)
% lufactor: Compute the LU decomposition of an n-by-n
% matrix A by direct factorization. On return, L is
% stored in the lower triangular part of A and U is
% stored in the upper triangular part.

   [n n] = size(A);
%                       Loop over the rows
   for i = 1: n - 1
%                       Calculate the i th column of L
      for j = i + 1: n
         for k = 1: i - 1
            A(j,i) = A(j,i) - A(j,k)*A(k,i);
         end
         A(j,i) = A(j,i)/A(i,i);
      end
%                       Calculate the (i + 1) th row of U
      for j = i+1: n
         for k = 1: i
            A(i+1,j) = A(i+1,j) - A(i+1,k)*A(k,j);
         end
      end
   end
```

LU Factorization

- **Observe:**
  i. The first row of $\mathbf{U}$ needs no explicit calculation
  ii. The 1s on the diagonal of $\mathbf{L}$ are not stored
  iii. MATLAB Loops do not execute when the lower index exceeds the upper one
  iv. Classical Gausian elimination corresponds to a different loop ordering
    – cf. Trefethen and Bau (1997), Lecture 20

- *Example 1.* Factor

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 0 & -4 \\ -1 & 0 & 6 & 2 \\ 3 & -2 & -25 & 0 \\ -2 & -3 & 4 & 4 \end{bmatrix}$$

  – $i = 1$: Calculate the first column of $\mathbf{L}$ and the second row of $\mathbf{U}$

$$\mathbf{A} \Rightarrow \begin{bmatrix} 1 & 2 & 0 & -4 \\ -1 & 2 & 6 & -2 \\ 3 & -2 & -25 & 0 \\ -2 & -3 & 4 & 4 \end{bmatrix}$$

LU Factorization

– $i = 2$: Calculate the second column of $\mathbf{L}$ and the third row of $\mathbf{U}$

$$\mathbf{A} \Rightarrow \begin{bmatrix} 1 & 2 & 0 & -4 \\ -1 & 2 & 6 & -2 \\ 3 & -4 & -1 & 4 \\ -2 & 1/2 & 4 & 4 \end{bmatrix}$$

– $i = 3$: Calculate the third column of $\mathbf{L}$ and the fourth row of $\mathbf{U}$

$$\mathbf{A} \Rightarrow \begin{bmatrix} 1 & 2 & 0 & -4 \\ -1 & 2 & 6 & -2 \\ 3 & -4 & -1 & 4 \\ -2 & 1/2 & -1 & 1 \end{bmatrix}$$

- The $\mathbf{L}$ and $\mathbf{U}$ factors

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 3 & -4 & 1 & 0 \\ -2 & 1/2 & -1 & 1 \end{bmatrix}, \qquad \mathbf{U} = \begin{bmatrix} 1 & 2 & 0 & -4 \\ 0 & 2 & 6 & -2 \\ 0 & 0 & -1 & 4 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

L Exposed

- Elementary transformations

$$\mathbf{L}_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ -3 & 0 & 1 & 0 \\ 2 & 0 & 0 & 1 \end{bmatrix}, \qquad \mathbf{L}_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 4 & 1 & 0 \\ 0 & -1/2 & 0 & 1 \end{bmatrix},$$

$$\mathbf{L}_3 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{bmatrix}$$

  - $\mathbf{L}_k$ is the identity matrix with its $k\ th$ column replaced by the $k\ th$ column of $\mathbf{L}$ with the negative of the subdiagonal elements

$$\mathbf{L}^{-1} = \mathbf{L}_3\mathbf{L}_2\mathbf{L}_1 \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 2.5 & 3.5 & 1 & 1 \end{bmatrix}$$

Forward and Backward Substitution

- Solution of (3b) by forward substitution

$$y_i = b_i - \sum_{j=1}^{i-1} l_{ij} y_j \tag{6a}$$

```
function y = forward(L, b)
% forward: Solution of a n-by-n lower triangular system
% Ly = b by forward substitution.

   [n n] = size(L);
   y(1) = b(1);
   for i = 2:n
      y(i) = b(i) - dot(L(i,1:i-1)', y(1:i-1));
   end
```

- Solve (3a) by backward substitution

$$x_i = \frac{1}{u_{ii}}[y_i - \sum_{j=i+1}^{n} u_{ij} x_j] \tag{6b}$$

```
function x = backward(U, y)
% backward: Solution of a n-by-n upper triangular system
% Ux = y by backward substitution.

   [n n] = size(U);
   x(n) = y(n)/U(n,n);
   for i = n - 1:-1:1
      x(i) = (y(i) - dot(U(i,i+1:n)', x(i+1:n)))/U(i,i);
   end
```

Forward and Backward Substitution

- *Example 2.* Solve the linear system $\mathbf{Ax} = \mathbf{b}$ for $\mathbf{x}$ when $\mathbf{A}$ is as given in Example 1 and

$$\mathbf{b} = [-1,\ 7,\ -24,\ 3]^T$$

  - Using the forward substitution algorithm

$$\mathbf{y} = [-1,\ 6,\ 3,\ 1]^T$$

  - Using backward substitution

$$\mathbf{x} = [1,\ 1,\ 1,\ 1]^T$$

Operation Count

- *Factorization:* (cf. p. 5)
  - Inner column loop:
    - $i-1$ multiplications and subtractions
    - 1 division
  - Inner row loop: i multiplications and subtractions
  - The summations on j give
    - $(2i-1)(n-i)$ multiplications and subtractions
    - $n-i$ divisions
  - The summations on i give
    - Multiplications and subtractions:

$$\sum_{i=1}^{n-1}(2i-1)(n-i) = \frac{n(n-1)(2n-1)}{6}$$

    - Divisions:

$$\sum_{i=1}^{n-1}(n-1) = \frac{n(n-1)}{2}$$

    - Formulas (1.2.1, 2) were used to obtain the result
  - A floating point operation (FLOP) is any $+, -, *, /, \sqrt{\ }, \cdots$
    - For large n the factorization has about $2n^3/3$ FLOPs

Operation Count

- *Forward Substitution*: (cf. p. 9)
  - $i-1$ multiplications and additions/subtractions in the dot product
    - Total multiplications and additions/subtractions:

$$\sum_{i=2}^{n}(i-1) = \frac{n(n-1)}{2}$$

- *Backward Substitution:*
  - $n(n-1)/2$ multiplications and additions/subtractions and n divisions
- *Forward and Backward Substitution*:
  - For large n, there are about $2n^2$ FLOPs
- Factorization dominates forward and backward substitution for large n

2.4. Pivoting

- Reading: Trefethen and Bau (1997), Lecture 21
- The Gaussian factorization and backward substitution fail when $u_{ii} = 0$, $i = 1 : n$
  - The system need not be singular, e.g.,

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$$

  - The factorization can proceed upon a row interchange
    - i.e., upon exchanging equations
  - Small divisors with finite-precision arithmetic will also cause problems
- *Example 1.* Consider three-decimal floating-point arithmetic ($\beta = 10$, $t = 3$)

$$\begin{bmatrix} 1.00 \times 10^{-4} & 1.00 \\ 1.00 & 1.00 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.00 \\ 2.00 \end{bmatrix}$$

  - The exact solution is $x_1 = 10000/9999 = 1.00010$ $x_2 = 9998/9999 = 0.99990$
  - Factorization:

$$\mathbf{L} = \begin{bmatrix} 1.00 & 0.00 \\ 1.00 \times 10^4 & 1.00 \end{bmatrix}$$

$$\mathbf{U} = \begin{bmatrix} 1.00 \times 10^{-}4 & 1.00 \\ 0.00 & -1.00 \times 10^4 \end{bmatrix}$$

The need for Pivoting

  - Forward substitution

$$\begin{bmatrix} 1.00 & 0.00 \\ 1.00 \times 10^4 & 1.00 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1.00 \\ 2.00 \end{bmatrix}$$

    or $y_1 = 1.00$, $y_2 = -1.00 \times 10^4$

  - Backward substitution

$$\begin{bmatrix} 1.00 \times 10^{-4} & 1.00 \\ 0.00 & -1.00 \times 10^4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.00 \\ -1.00 \times 10^4 \end{bmatrix}$$

  - Thus, $x_2 = 1.00$, $x_1 = 0.00$

- This is awful!
- Interchanging rows

$$\begin{bmatrix} 1.00 & 1.00 \\ 0.00 & 1.00 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 2.00 \\ 1.00 \end{bmatrix}$$

  - The system is in upper triangular form ($l_{21} = 0.00$), so $x_2 = 1.00$ and $x_1 = 1.00$
    * This is correct to three digits

Pivoting Strategies

- Row pivoting (partial pivoting): at stage i of the outer loop of the factorization (cf. Section 2.3, p. 5)
  1. Find r such that $|a_{ri}| = \max_{i \le k \le n} |a_{ki}|$
  2. Interchange rows i and r
- Column pivoting: Proceed as row pivoting but interchange columns
  - Column pivoting requires reordering the unknowns
  - Column pivoting does not work well with direct factorization
- Complete pivoting: Choose r and c such that
  1. Find $r,\ c$ such that $|a_{rc}| = \max_{i \le k,l \le n} |a_{kl}|$
  2. Interchange rows i and r and columns i and c
- Complete pivoting is less common than partial pivoting
  - Have to search a larer space
  - Have to reorder unknowns
- Row pivoting is usually adequate
- Row, column, and complete pivoting have $l_{ij} \le 1$, $i \ne j$

Scaled Partial Pivoting

- The equations and unknowns may be scaled differently
- *Example 2.* Multiply the first row of Example 1 by 10^5

$$\begin{bmatrix} 1.00 \times 10^1 & 1.00 \times 10^5 \\ 1.00 & 1.00 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1.00 \times 10^5 \\ 2.00 \end{bmatrix}$$

  - Row pivoting would choose the first row as a pivot
    - This yields the result $x_2 = 1.00$ and $x_1 = 0.00$
- There is no general solution to this problem
  - One strategy is to "equilibrate" the matrix
    - Select all elements to have the same magnitude
- Scaled partial pivoting:
  - Select row pivots relative to the size of the row
    1. Before factorization select scale factors

$$s_i = \max_{1 \le j \le n} |a_{ij}|, \qquad i = 1 : n$$

    2. At stage i of the factorization, select r such that

$$\left| \frac{a_{ri}}{s_r} \right| = \max_{i \le k \le n} \left| \frac{a_{ki}}{s_k} \right|$$

    3. Interchange rows k and i

Factorization with Pivoting

- Gaussian elimination with partial pivoting always finds factors $\mathbf{L}$ and $\mathbf{U}$ of a nonsingular matrix
  - Neglecting roundoff errors
- **Theorem 1**: For any $n \times n$ matrix $\mathbf{A}$ of rank n, there is a reordering of rows such that

$$\mathbf{PA} = \mathbf{LU} \tag{1}$$

  where $\mathbf{P}$ is a permutation matrix that reorders the rows of $\mathbf{A}$
  - A permutation matrix is an identity matrix with its rows or columns interchanged
  - *Proof:* cf. Golub and Van Loan (1996), Section 3.4.4 □

Scaled Partial Pivoting

- It is not necessary to store the permutation matrix or rearrange the rows of $\mathbf{A}$
  - Row interchanges can be recorded in a vector $\mathbf{p}$
- *Example 3.* Consider

$$\mathbf{A} = \begin{bmatrix} 1 & -1 & 2 \\ 1 & -1 & 1 \\ 2 & 3 & -1 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix}$$

  - Compute the scale factors and initialize the interchange vector

$$\mathbf{s} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}, \qquad \mathbf{p} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

    * $p_i = i$, $i = 1 : n$, implies no rows have been interchanged
  - $i = 1$:
    * Scale factor: $|a_{11}/s_1| = 1/2, |a_{21}/s_2| = 1/1, |a_{31}/s_3| = 2/3$
    * The second row is the pivot

$$\mathbf{s} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}, \qquad \mathbf{A} \Rightarrow \begin{bmatrix} 1 & 0 & 1 \\ 1 & -1 & 1 \\ 2 & 5 & -3 \end{bmatrix}, \qquad \mathbf{p} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

  - $\mathbf{p}$ records the implicit row interchange

Scaled Partial Pivoting

– $i = 2$:

  * Scale factors: $|a_{12}/s_1| = 0/2$, $|a_{32}/s_3| = 5/3$
  * The third row is the pivot

$$\mathbf{s} = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}, \qquad \mathbf{A} \Rightarrow \begin{bmatrix} 1 & 0 & 1 \\ 1 & -1 & 1 \\ 2 & 5 & -3 \end{bmatrix}, \qquad \mathbf{p} = \begin{bmatrix} 2 \\ 3 \\ 1 \end{bmatrix}$$

– Construct $\mathbf{P}$, $\mathbf{L}$, and $\mathbf{U}$

  * $p_1 = 2$, so Row 1 of $\mathbf{L}$ and $\mathbf{U}$ is Row 2 of $\mathbf{A}$
  * $p_2 = 3$, so Row 2 of $\mathbf{L}$ and $\mathbf{U}$ is Row 3 of $\mathbf{A}$
  * $p_3 = 1$, so Row 3 of $\mathbf{L}$ and $\mathbf{U}$ is Row 1 of $\mathbf{A}$

$$\mathbf{L} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \qquad \mathbf{U} = \begin{bmatrix} 1 & -1 & 1 \\ 0 & 5 & -3 \\ 0 & 0 & 1 \end{bmatrix}$$

  * From $\mathbf{p}$, Row 1 of $\mathbf{P}$ is Row 2 of the identity matrix
  * Row 2 of $\mathbf{P}$ is Row 3 of the identity matrix
  * Row 3 of $\mathbf{P}$ is Row 1 of the identity matrix

$$\mathbf{P} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Scaled Partial Pivoting

- Check that $\mathbf{PA} = \mathbf{LU}$

$$\mathbf{PA} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & -1 & 2 \\ 1 & -1 & 1 \\ 2 & 3 & -1 \end{bmatrix} =$$

$$\mathbf{LU} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & -1 & 1 \\ 0 & 5 & -3 \\ 0 & 0 & 1 \end{bmatrix} =$$

- Forward and backward substition.

$$\mathbf{PAx} = \mathbf{Pb}$$

  - Use (1)

$$\mathbf{LUx} = \mathbf{Pb}$$

- Forward substitution: $\mathbf{Ly} = \mathbf{Pb}$
  - $\mathbf{p}_1 = 2$, so $y_1 = b_2 = 1$ or $y_1 = 1$
  - $\mathbf{p}_2 = 3$, so $2y_1 + y_2 = b_3 = 4$ or $y_2 = 2$
  - $\mathbf{p}_3 = 1$, so $y_1 + y_3 = b_1 = 2$ or $y_3 = 1$
- Backward substitution: $\mathbf{Ux} = \mathbf{y}$
  - $\mathbf{p}_3 = 1$, so $x_3 = y_3 = 1$ or $x_3 = 1$
  - $\mathbf{p}_2 = 3$, so $5x_2 - 3x_3 = y_2 = 2$ or $x_2 = 1$
  - $\mathbf{p}_1 = 2$, so $x_1 - x_2 + x_3 = y_1 = 1$ or $x_1 = 1$

LU Factorization

```
function [Ap] = plufactor(A)
% plufactor: Factor the n-by-n matrix A into LU. On return, L – I
% is stored in the lower triangular part of A and U
% is stored in the upper triangular part. The vector p
% stores the permuted row indices using scaled partial pivoting.

   [n n] = size(A);
%                          Initialize p and compute the scale vector s
   for i = 1; n
      s(i) = norm(A(i,1:n), inf);
      p(i) = i;
   end
%                          Loop over the rows
   for i = 1: n - 1
%                          Find the best pivot row
      colmax = 0;
      for k = i: n
         srow = abs(A(p(k),i))/s(p(k));
         if colmax < srow;
            colmax = srow;
            index = k;
         end
      end
      temp = p(i);
      p(i) = index;
      p(index) = temp;
%                          Calculate the i th column of L
      for j = i + 1: n
         for k = 1: i - 1
            A(p(j),i) = A(p(j),i) - A(p(j),k)*A(p(k),i);
         end
         A(p(j),i) = A(p(j),i)/A(p(i),i);
      end
%                          Calculate the (i + 1) th row of U
      for j = i+1: n
         for k = 1: i
            A(p(i+1),j) = A(p(i+1),j) - A(p(i+1),k)*A(p(k),j);
         end
      end
   end
```

Forward and Backward Substitution

```
function y = pforward(L, b, p)
% pforward: Solution of a n-by-n lower triangular system
% Ly = Pb by forward substitution. Row permutations have been
% stored in the vector p.

   [n n] = size(L);
   y(1) = b(p(1));
   for i = 2:n
      y(i) = b(p(i)) - dot(L(p(i),1:i-1)', y(1:i-1));
   end
```

```
function x = backward(U, y, p)
% pbackward: Solution of a n-by-n upper triangular system
% Ux = y by backward substitution. Row permuations have been
% stored in the vector p.

   [n n] = size(U);
   x(n) = y(n)/U(p(n),n);
   for i = n - 1: -1: 1
      x(i) = (y(i) - dot(U(p(i),i+1:n)', x(i+1:n)))/U(p(i),i);
   end
```

- **Note**:

  i. No attempt has been made to check for failure

     – **A** is singular if $colmax = 0$ or $s_i = 0$ for some i

  ii. The MATLAB function *norm* computes vector and matrix norms.

2.5. Accuracy Estimation

- Reading: Trefethen and Bau (1997), Lecture 22
- *Accuracy:*
  - With roundoff, how accurate is a solution obtained by Gaussian elimination?
  - How sensitive is a solution to perturbations introduced by round off error (stability)?
  - How can we appraise the accuracy of a computed solution?
  - Can the accuracy of a computed solution be improved?
- Let $\hat{\mathbf{x}}$ be a computed solution of

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1}$$

  - Compute the residual

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\hat{\mathbf{x}} \tag{2}$$

  - Is $\mathbf{r}$ a good measure of the accuracy of $\hat{\mathbf{x}}$?
- *Example 1.* Solve (1) with

$$\mathbf{A} = \begin{bmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 0.8642 \\ 0.1440 \end{bmatrix}$$

  - An approximate solution is $\hat{\mathbf{x}} = [0.9911, -0.4870]^T$
  - The residual is $\mathbf{r} = [-10^{-8}, 10^{-8}]^T$
  - Exact solution:
  - $\det(\mathbf{A}) = 10^{-8}$

Sensitivity

- *Example 2.* Consider

$$\mathbf{A} = \begin{bmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{bmatrix}$$

  - $\mathbf{A}$ is symmetric and positive definite with $\det(\mathbf{A}) = 1$
  - Exact solutions

$\mathbf{b}^T$	$\mathbf{x}^T$
$[23, 32, 33, 31]$	$[1, 1, 1, 1]$
$[22.9, 32.1, 32.9, 31.1]$	$[-7.2, 6, 2.9, 0.1]$
$[22.99, 32.01, 32.99, 31.01]$	$[0.18, 1.5, 1.19, 0.89]$

Perturbations

- **Definition 1**: A matrix is *ill-conditioned* if small changes in $\mathbf{A}$ or $\mathbf{b}$ produce large changes in the solution.
  - Suppose that $\mathbf{b}$ is perturbed to $\boldsymbol{b} + \boldsymbol{\delta b}$
  - The solution $\boldsymbol{x} + \boldsymbol{\delta x}$ of the perturbed system would satisfy
$$\mathbf{A}(\mathbf{x} + \boldsymbol{\delta x}) = \mathbf{b} + \boldsymbol{\delta b}$$
  - Estimate the magnitude of $\boldsymbol{\delta x}$
$$\boldsymbol{\delta x} = \mathbf{A}^{-1}\boldsymbol{\delta b}$$
  - Taking a norm
$$||\boldsymbol{\delta x}|| = ||\mathbf{A}^{-1}\boldsymbol{\delta b}|| \leq ||\mathbf{A}^{-1}||||\boldsymbol{\delta b}||$$
  - In addition
$$||\mathbf{b}|| = ||\mathbf{A}\mathbf{x}|| \leq ||\mathbf{A}||^{|}|\mathbf{x}||$$
  - Multiplying the two inequalities
$$||\boldsymbol{\delta x}||||\mathbf{b}|| \leq ||\mathbf{A}||||\mathbf{A}^{-1}||||\boldsymbol{\delta b}||^{|}|\mathbf{x}||$$
    or
$$\frac{||\boldsymbol{\delta x}||}{||\mathbf{x}||} \leq \kappa(\mathbf{A})\frac{||\boldsymbol{\delta b}||}{||\mathbf{b}||} \tag{3a}$$
    where
$$\kappa = ||\mathbf{A}||||\mathbf{A}^{-1}|| \tag{3b}$$
    * $\kappa(\mathbf{A})$ is called the *condition number*

The Condition Number

- **Note**:

  i. The condition number relates the relative uncertainty of the data ($||\boldsymbol{\delta b}||/||\mathbf{b}||$) to the relative uncertainty of the solution ($||\boldsymbol{\delta x}||/||\mathbf{x}||$)

  ii. If $\kappa(\mathbf{A})$ is large, small changes in $\mathbf{b}$ may result in large changes in $\mathbf{x}$

  iii. If $\kappa(\mathbf{A})$ is large, $\mathbf{A}$ is *ill-conditioned*

  iv. The bound (3a) is sharp: there are $\mathbf{b}$s for which equality holds

  v. The $\det(\mathbf{A})$ has nothing to do with conditioning. The matrix

$$\begin{bmatrix} 10^{-30} & 0 \\ 0 & 10^{-30} \end{bmatrix}$$

  is well-conditioned

- Repeat the analysis for a perturbation in $\mathbf{A}$

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

or

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

or

$$\boldsymbol{\delta x} = -\mathbf{A}^{-1}\boldsymbol{\delta A}(\mathbf{x} + \boldsymbol{\delta x})$$

or

$$||\boldsymbol{\delta x}|| \leq ||\mathbf{A}^{-1}||||\boldsymbol{\delta A}||||\mathbf{x} + \boldsymbol{\delta x}||$$

or

$$\frac{||\boldsymbol{\delta x}||}{||\mathbf{x} + \boldsymbol{\delta x}||} \leq \kappa(\mathbf{A})\frac{||\boldsymbol{\delta A}||}{||\mathbf{A}||} \tag{3c}$$

Condition Numbers

- *Example 3.* The matrix $\mathbf{A}$ of Example 1 and its inverse are

$$\mathbf{A} = \begin{bmatrix} 1.2969 & 0.8648 \\ 0.2161 & 0.1441 \end{bmatrix}, \qquad \mathbf{A}^{-1} = 10^8 \begin{bmatrix} 0.1441 & -0.8648 \\ -0.2161 & 1.2969 \end{bmatrix}$$

  – Calculate

$$||\mathbf{A}||_\infty = 2.1617, \qquad ||\mathbf{A}^{-1}||_\infty = 1.5130 \times 10^8$$

$$\kappa_\infty(\mathbf{A}) = 3.2707 \times 10^8$$

- *Example 4.* The matrix $\mathbf{A}$ of Example 2 and its inverse are

$$\mathbf{A} = \begin{bmatrix} 5 & 7 & 6 & 5 \\ 7 & 10 & 8 & 7 \\ 6 & 8 & 10 & 9 \\ 5 & 7 & 9 & 10 \end{bmatrix}, \qquad \mathbf{A}^{-1} = \begin{bmatrix} 68 & -41 & -17 & 10 \\ -41 & 25 & 10 & -6 \\ -17 & 10 & 5 & -3 \\ 10 & -6 & -3 & 2 \end{bmatrix}$$

  and

$$||\mathbf{A}||_\infty = 33, \qquad ||\mathbf{A}^{-1}||_\infty = 136$$

$$\kappa_\infty(\mathbf{A}) = 4488$$

Stability of Gaussian Elimination

- How do rounding errors propagate in Gaussian elimination?
  - Let's discuss this without explicit treatment of pivoting
    - Assume that $\mathbf{A}$ has its rows arranged so that pivoting is unnecessary

- **Theorem 1**: Let $\mathbf{A}$ be an $n \times n$ real matrix of floating-point numbers on a computer with unit round-off error u. Assume that no zero pivots are encountered. Let $\hat{\mathbf{L}}$ and $\hat{\mathbf{U}}$ be the computed triangular factors of $\mathbf{A}$ and let $\hat{\mathbf{y}}$ and $\hat{\mathbf{x}}$ be the computed solutions of

$$\hat{\mathbf{L}}\mathbf{y} = \mathbf{b}, \qquad \hat{\mathbf{U}}\mathbf{x} = \hat{\mathbf{y}} \tag{4a}$$

  Then

$$(\mathbf{A} + \boldsymbol{\delta A})\hat{\mathbf{x}} = \mathbf{b} \tag{4b}$$

  where

$$|\boldsymbol{\delta A}| \leq 3nu|\mathbf{L}||\mathbf{U}| + O(n^2u^2) \tag{4c}$$

  - *Remark 1*: Recall (Section 2.1) that $|\mathbf{A}|$ is a matrix with elements $|a_{ij}|$, $i, j = 1 : n$
  - *Remark 2*: The computed solution $\hat{\mathbf{x}}$ is the exact solution of a system $\mathbf{A} + \boldsymbol{\delta A}$
  - *Remark 3*: Additionally, $\hat{\mathbf{L}}$ and $\hat{\mathbf{U}}$ are the exact factors of a perturbed matrix $\mathbf{A} + \mathbf{E}$

- *Proof:* Follow the arguments used in the round-off error analysis of the dot product of Section 2.1 (cf. Demmel, Section 2.4) $\square$

Growth Factor

- *Remark*: For the infinity, one and Frobenius norms,

$$|| \, |\mathbf{z}| \, || = ||\mathbf{z}||$$

  - Taking a norm of (4c)

$$||\boldsymbol{\delta A}|| \leq 3nu||\mathbf{L}||||\mathbf{U}|| + O(n^2u^2) \tag{5}$$

- We would like to estimate $||\mathbf{L}||$ and $||\mathbf{U}||$
  - With partial pivoting, the elements of $\mathbf{L}$ are bounded by unity
    - Thus, $||\mathbf{L}||_\infty \leq n$
  - Bounding $||\mathbf{U}||$ is much more difficult
    - Define the *growth factor* as

$$\rho = \frac{\max_{i,j} |u|_{ij}}{||\mathbf{A}||_\infty} \tag{6}$$

    - Then $|\mathbf{U}| \leq \rho||\mathbf{A}||$ and

$$||\mathbf{U}||_\infty \leq \rho n||\mathbf{A}||_\infty$$

  - Using the bounds for $||\mathbf{L}||_\infty$ and $||\mathbf{U}||_\infty$ in (5), we find

$$||\boldsymbol{\delta A}||_\infty \leq n^3 u\rho C||\mathbf{A}||_\infty \tag{7}$$

    - The constant C accounts for our "casual" treatment of the $O(n^2u^2)$ term

Growth Factors

- **Note**:

  i. The bound (7) for $\boldsymbol{\delta A}$ is acceptable unless ρ is large

  ii. J.H. Wilkinson (1961) [1] shows that if $|a_{ij}| \leq 1$, $i, j = 1 : n$,

  - $\rho||\mathbf{A}||_\infty \leq 2^{n-1}$ with partial pivoting
  - $\rho||\mathbf{A}||_\infty \leq 1.8n^{0.25 \ln n}$ with complete pivoting
  - The bound with partial pivoting is sharp! Consider

$$\mathbf{A} = \begin{bmatrix} 1 & & & & 1 \\ -1 & 1 & & & 1 \\ -1 & -1 & 1 & & 1 \\ -1 & -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix}$$

  which has

$$\mathbf{L} = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & 1 & & \\ -1 & -1 & -1 & 1 & \\ -1 & -1 & -1 & -1 & 1 \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} 1 & & & & 1 \\ & 1 & & & 2 \\ & & 1 & & 4 \\ & & & 1 & 8 \\ & & & & 16 \end{bmatrix}$$

  Thus, $\rho = 16$. For an $n \times n$ matrix, $\rho = 2^{n-1}$

  iii. In most cases, $\rho||\mathbf{A}||_\infty \leq 8$ with partial pivoting

  iv. Our bounds are conservative. In most cases

$$||\boldsymbol{\delta A}||_\infty \leq nu||\mathbf{A}||_\infty$$

[1] J.H. Wilkinson, "Error analysis of direct methods of matrix inversion," *J. A.C.M.*, **8**, 281-330

Iterative Improvement

- Iterative improvement can enhance the accuracy of a computed solution
  - It works best when double precision arithmetic is available but costs much more than single precision arithmetic
- Let $\hat{\mathbf{x}}$ be an approximate solution of (1).
- Calculate the residual (2)

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\hat{\mathbf{x}} = \mathbf{A}(\mathbf{x} - \hat{\mathbf{x}})$$

- Solve

$$\boldsymbol{A\delta x} = \mathbf{r} \tag{8a}$$

  for $\boldsymbol{\delta x}$ and calculate an "improved" solution

$$\mathbf{x} = \hat{\mathbf{x}} + \boldsymbol{\delta x} \tag{8b}$$

- $\hat{\mathbf{x}}$ cannot be improved unless:
  - The residual is calculated in double precision
  - The original (not the factored) $\mathbf{A}$ is used to calculate $\mathbf{r}$
- The procedure is
  1. Calculate $\mathbf{r} = \mathbf{b} - \mathbf{A}\hat{\mathbf{x}}$ using double precision
  2. Solve $\hat{\mathbf{L}}\mathbf{y} = \mathbf{Pr}$ by forward substitution
  3. Solve $\hat{\mathbf{U}}\boldsymbol{\delta x} = \mathbf{y}$ by backward substitution
  4. $\mathbf{x} = \hat{\mathbf{x}} + \delta\mathbf{x}$

Iterative Improvement

- **Notes:**
  i. Round the double precision residual to single precision
  ii. The cost of iterative improvement:
    - One matrix-by-vector multiplication for the residual and one forward and backward substitution
    - Each cost n^2 multiplications if double precision hardware is available
    - The total cost of $2n^2$ multiplications is small relative to the factorization
  iii. Continue the iteration for further improvement
  iv. Have to save the original $\mathbf{A}$ and the factors $\hat{\mathbf{L}}$ and $\hat{\mathbf{U}}$
  v. Have to do mixed-precision arithmetic

- Accuracy of the improved solution
  - From (8)
$$\boldsymbol{\delta x} := \mathbf{x} - \hat{\mathbf{x}} = \mathbf{A}^{-1}(\mathbf{b} - \mathbf{A}\hat{\mathbf{x}}) = \mathbf{A}^{-1}\mathbf{r}$$
  - Take a norm
$$||\boldsymbol{\delta x}||_\infty \leq ||\mathbf{A}^{-1}||_\infty ||\mathbf{r}||_\infty$$
  - $\hat{\mathbf{x}}$ satisfies (4c), so
$$\mathbf{r} = (\mathbf{A} + \boldsymbol{\delta A})\hat{\mathbf{x}} - \mathbf{A}\hat{\mathbf{x}} = \boldsymbol{\delta A}\hat{\mathbf{x}}$$
  - Take a norm
$$||\mathbf{r}||_\infty \leq ||\boldsymbol{\delta A}||_\infty ||\hat{\mathbf{x}}||_\infty$$

Still Improving

- Combining results

$$||\boldsymbol{\delta x}||_\infty \leq ||\mathbf{A}^{-1}||_\infty ||\boldsymbol{\delta A}||_\infty ||\hat{\mathbf{x}}||_\infty$$

- Using (3b)

$$\frac{||\boldsymbol{\delta x}||_\infty}{||\hat{\mathbf{x}}||_\infty} \leq \kappa(\mathbf{A}) \frac{||\boldsymbol{\delta A}||_\infty}{||\mathbf{A}||_\infty} \tag{9a}$$

- We could estimate $||\boldsymbol{\delta A}||_\infty$ using (7)
  - Golub and Van Loan (1996) suggest

$$||\boldsymbol{\delta A}||_\infty = nu||\mathbf{A}||_\infty$$

  - Trefethen and Bau (1997) suggest $\rho = O(n^{1/2})$

$$\frac{||\boldsymbol{\delta x}||_\infty}{||\hat{\mathbf{x}}||_\infty} \leq nu\kappa(\mathbf{A}) \tag{9b}$$

- If $u \propto \beta^{1-t}$ and $\kappa(\mathbf{A}) \propto \beta^{s-1}$

$$\frac{||\boldsymbol{\delta x}||_\infty}{||\hat{\mathbf{x}}||_\infty} \leq nc\beta^{s-t} \tag{9c}$$

  - c represents constants arising from u and κ

- The computed solution $\hat{\mathbf{x}}$ will have about $t-s$ correct β-digits
  - If s is small, $\mathbf{A}$ is well conditioned and the error is small
  - If s is large, $\mathbf{A}$ is ill-conditioned and the error is large
  - If $s > t$, the error grows relative to $\hat{\mathbf{x}}$

It Don't Get Much Better

- Let $\hat{\mathbf{x}}^{(0)} = \hat{\mathbf{x}}$, $\boldsymbol{\delta x}^{(0)} = \boldsymbol{\delta x}$, and $\hat{\mathbf{x}}^{(1)} = \hat{\mathbf{x}}^{(0)} + \boldsymbol{\delta x}^{(0)}$ be the solution computed by iterative improvement.
- Assume $\boldsymbol{\delta x} \approx \boldsymbol{\delta x}^{(0)}$ and Calculate an estimate of $\kappa(\mathbf{A})$ from (9b) as

$$\frac{1}{nu}\frac{||\boldsymbol{\delta x}^{(0)}||_\infty}{||\hat{\mathbf{x}}^{(0)}||_\infty} \leq \kappa(\mathbf{A})$$

- An empirical result that holds widely is

$$\frac{1}{n}\kappa(\mathbf{A}) \leq \frac{1}{nu}\frac{||\boldsymbol{\delta x}^{(0)}||_\infty}{||\hat{\mathbf{x}}||_\infty} \leq \kappa(\mathbf{A}) \tag{10}$$

- **Theorem 2**: Suppose

$$\mathbf{r}^{(k)} = \mathbf{b} - \mathbf{A}\hat{\mathbf{x}}^{(k)}, \qquad \hat{\mathbf{x}}^{(k+1)} = \mathbf{x}^{(k)} + \boldsymbol{\delta x}^{(k)} \tag{11}$$

  are calculated in double precision and $\boldsymbol{\delta x}^{(k)}$ is the solution of

$$\mathbf{A}\boldsymbol{\delta x}^{(k)} = \mathbf{r}^{(k)}$$

  in single precision. Thus,

$$(\mathbf{A} + \boldsymbol{\delta A}^{(k)})\boldsymbol{\delta x}^{(k)} = \mathbf{r}^{(k)}$$

  If $||\mathbf{A}^{-1}\boldsymbol{\delta A}^{(k)}|| \leq 1/2$ then $||x^{(k)} - \mathbf{x}|| \to 0$ as $k \to \infty$
- **Corollary 2**: If $||\boldsymbol{\delta A}^{(k)}|| \leq nu||\mathbf{A}||$ and $nu\kappa(\mathbf{A}) \leq 1/2$ then $||\mathbf{x}^{(k)} - \mathbf{x}|| \to 0$ as $k \to \infty$
  - *Proof*: cf. G.E. Forsythe and C. Moler (1967), *Computer Solution of Linear Algebraic Systems*, Prentice Hall, Englewood Cliffs.
- *Remark*: Iterative improvement converges rather generally and each iteration gives $t - s$ correct β digits

A Hilbert Matrix

- *Example 5.* An $n \times n$ Hilbert matrix has entries

$$h_{ij} = \frac{1}{i + j - 1}$$

  - With $n = 4$:

$$\mathbf{H} = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}$$

  - It is symmetric and positive definite
  - It arises in the polynomial approximation of functions

- Condition numbers of Hilbert matrices

n	$\kappa_2(\mathbf{H})$
2	1.9282e+01
4	1.5514e+04
8	1.5258e+10
16	6.5341e+17

- Solve $\mathbf{Hx} = \mathbf{b}$ with $n = 12$
  - Select $\mathbf{b}$ the first column of the identity matrix
  - $\mathbf{x}$ is the first column of $\mathbf{H}^{-1}$

- Solve by Gaussian elimination with one step of iterative improvement

$$\frac{||\hat{\mathbf{x}}^{(0)} - \mathbf{x}||_2}{||\mathbf{x}||_2} = 0.0784, \qquad \frac{||\hat{\mathbf{x}}^{(1)} - \mathbf{x}||_2}{||\mathbf{x}||_2} = 0.0086$$

3. Special Linear Systems
3.1. Symmetric Positive Definite Systems

- Reading: Trefethen and Bau (1997), Lecture 23
- Simplify Gaussian elimination when $\mathbf{A}$ has special properties
  - Symmetry
  - positive definiteness
  - Banded structure
  - Sparsity
  - Block structure
- **Definition 1:** $\mathbf{A} \in \Re^{n \times n}$ is symmetric if $\mathbf{A}^T = \mathbf{A}$
- **Definition 2:** $\mathbf{A} \in \Re^{n \times n}$ is *positive definite* if $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$ for all nonzero $\mathbf{x} \in \Re^n$
- If $\mathbf{A}$ is positive definite:
  - and $\mathbf{X} \in \Re^{n \times k}$ has rank k then $\mathbf{X}^T \mathbf{A} \mathbf{X}$ is positive definite
  - then all of its principal submatrices are positive definite
  - then all of its diagonal entries are positive
  - then it may be factored as

    $$\mathbf{A} = \mathbf{L}\mathbf{U} = \mathbf{L}\mathbf{D}\mathbf{M}^T$$

    where $\mathbf{L}$ and $\mathbf{M}$ are unit lower triangular and $\mathbf{D}$ is diagonal with positive entries
    - The entries of $\mathbf{D}$ are the diagonal entries of $\mathbf{U}$
  - These properties are proved in Golub and Van Loan (1993), Section 4.2 or Demmel (1997), Section 2.7

Symmetric Positive Definite Systems

- Symmetric positive definite systems:
  - Arise in the finite difference or finite element solution of elliptic PDEs
  - $\mathbf{A}$ may be factorized as

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^T \tag{1a}$$

with

$$\mathbf{L} = \begin{bmatrix} 1 & & & \\ l_{21} & 1 & & \\ l_{31} & l_{32} & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & & 1 \end{bmatrix}, \qquad \mathbf{D} = \begin{bmatrix} d_1 & & & \\ & d_2 & & \\ & & \ddots & \\ & & & d_n \end{bmatrix} \tag{1b}$$

    - Zero entries are not shown

  - By direct factorization without pivoting

$$d_j = a_{jj} - \sum_{k=1}^{j-1} d_k l_{jk}^2, \tag{2a}$$

$$l_{ij} = \frac{1}{d_j}(a_{ij} - \sum_{k=1}^{j-1} d_k l_{jk} l_{ik}), \qquad i = j+1 : n, \quad j = 1 : n \tag{2b}$$

    - Summations are zero when the lower limit exceeds the upper one

Symmetric Positive Definite Factorization

```
function A = ldlt(A)
% ldlt: Factorization of a symmetric positive definite n-by-n
% matrix A into the product LDL', where L
% is unit lower triangular and D is diagonal. On return,
% A(i,j) stores L(i,j) if i > j and D(i) if i = j.

   [n n] = size(A);
   for j = 1:n
%                          Compute v(k), k = 1: j - 1
      for k = 1: j - 1
         v(k) = A(j,k)*A(k,k);
      end
%                          Compute d(j)
      v(j) = A(j,j) - dot(A(j,1:j-1),v(1:j-1));
      A(j,j) = v(j);
%                          Compute l(i,j), i = j + 1: n
      for i = j + 1:n
         A(i,j) = (A(i,j) - dot(A(i,1:j-1),v(1:j-1)))/v(j);
      end
   end
```

- We let $v_k = d_k l_{jk}$, $k = 1 : j - 1$
- We should use a symmetric storage mode, cf. Section 1.2
- The algorithm requires approximately $n^3/3$ FLOPs (half that of Gaussian elimination)
- Pivoting is not necessary for stability

Forward and Backward Substitution

- From (1a)

$$\mathbf{Ax} = \mathbf{LDL}^T\mathbf{x} = \mathbf{b}$$

  - Let

$$\mathbf{L}^T\mathbf{x} = \mathbf{y}, \qquad \mathbf{Dy} = \mathbf{z}, \qquad \mathbf{Lz} = \mathbf{b} \tag{3}$$

  - Forward substitution:

$$z_i = b_i - \sum_{k=1}^{i-1} l_{ik} z_k, \qquad i = 1 : n \tag{4a}$$

  - Diagonal scaling

$$y_i = z_i / d_i, \qquad i = 1 : n \tag{4b}$$

  - Backward substitution

$$x_i = y_i - \sum_{k=i+1}^{n} l_{ki} x_k, \qquad i = n : -1 : 1 \tag{4c}$$

- *Cholesky Factorization:*

$$\mathbf{A} = \tilde{\mathbf{L}}\tilde{\mathbf{L}}^T, \qquad \tilde{\mathbf{L}} = \mathbf{L}\mathbf{D}^{1/2}$$

  - The diagonal entries of $\tilde{\mathbf{L}}$ are square roots of the entires of $\mathbf{D}$
  - cf. Trefethen and Bau (1997), Lecture 23
  - The n square roots may be expensive

3.2. Banded and Profile Systems

- If $\mathbf{A} \in \Re^{n \times n}$ has lower bandwidth p and upper bandwidth q then
  - $\mathbf{L}$ has lower bandwidth p
    - $l_{ij} = 0$ for $j > i$ and $i > j + p$
  - $\mathbf{U}$ has upper bandwidth q
    - $u_{ij} = 0$ for $i > j$ and $j > i + q$
- *Example 1.* A 6×6 matrix with $p = 2$ and $q = 1$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & & & & \\ a_{21} & a_{22} & a_{23} & & & \\ a_{31} & a_{32} & a_{33} & a_{34} & & \\ & a_{42} & a_{43} & a_{44} & a_{45} & \\ & & a_{53} & a_{54} & a_{55} & a_{56} \\ & & & a_{64} & a_{65} & a_{66} \end{bmatrix}$$

  - Zeros are not shown

$$\mathbf{LU} = \begin{bmatrix} 1 & & & & & \\ l_{21} & 1 & & & & \\ l_{31} & l_{32} & 1 & & & \\ & l_{42} & l_{43} & 1 & & \\ & & l_{53} & l_{54} & 1 & \\ & & & l_{64} & l_{65} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & & & & \\ & u_{22} & u_{23} & & & \\ & & u_{33} & u_{34} & & \\ & & & u_{44} & u_{45} & \\ & & & & u_{55} & u_{56} \\ & & & & & u_{66} \end{bmatrix}$$

LU Factorization

- Linear equations solution
  - Use direct factorization
  - Neglect pivoting
    - Dangerous unless $\mathbf{A}$ is symmetric and positive definite
- *Factorization:*
  - u_{ij} and l_{ij} involve inner products between
    - the ith row of $\mathbf{L}$
    - the jth column of $\mathbf{U}$
    - l_{ij} is nonzero for $\max(1, i-p) \le j \le i$
    - u_{ij} is nonzero for $\max(1, j-q) \le i \le j$
  - Let

$$k^* = \max(1, i-p, j-q) \tag{1a}$$

$$u_{ij} = a_{ij} - \sum_{k=k^*}^{i-1} l_{ik} u_{kj}, \qquad j = i : i+q, \tag{1b}$$

$$l_{ji} = \frac{1}{u_{ii}}(a_{ji} - \sum_{k=k^*}^{i-1} l_{jk} u_{ki}), \qquad j = i+1 : i+p, \quad i = 1 : n \tag{1c}$$

    - A procedure should use the banded data structure of Section 1.2

Forward and Backward Substitution

- *Forward substitution:*

$$y_i = b_i - \sum_{k=\max(1,i-p)}^{i-1} l_{ik} y_k, \qquad i = 1 : n \tag{2a}$$

- *Backward substitution:*

$$x_i = \frac{1}{u_{ii}}(y_i - \sum_{k=i+1}^{\min(n,i+q)} u_{ik} y_k), \qquad i = n : -1 : 1 \tag{2b}$$

- *Operations and Storage* (with $p = q$):
  - Storage is $2(p+1)(n-p/2)$ locations
  - Factorization with $n \gg 1$, $p/n \ll 1$
    - Each inner product requires $i - k^*$ multiplications and subtractions and one division
    - $k^* = i - p$ for most rows
    - Summing on i, there are approximately $np(2p+1)$ multiplications and subtractions and np divisions
    - Thus, there are approximately $np(4p+3)$ FLOPs
  - Forward and backward substitution
    - There are approximately $2np$ multiplications and subtractions and n divisions or $n(4p+1)$ FLOPs
  - A full matrix requires about $2n^3/3$ FLOPs to factor and $2n^2$ to solve

Symmetric Positive Definite Band Matrices

- Let $\mathbf{A}$ be symmetric and positive definite with $p = q$
  - *Factorization* (cf. (1.2)):

$$k^* = \max(1, i - p)$$

$$d_j = a_{jj} - \sum_{k=k^*}^{j-1} d_k l_j k^2, \tag{3a}$$

$$l_{ij} = \frac{1}{d_j}(a_{ij} - \sum_{k=k^*}^{j-1} d_k l_{jk} l_{ik}), \qquad i = j+1 : j+p, \quad j = 1 : n \tag{3b}$$

  - *Forward substitution:*

$$z_i = b_i - \sum_{k=\max(1,i-p)}^{i-1} l_{ik} z_k, \qquad i = 1 : n \tag{4a}$$

  - *Diagonal scaling:*

$$y_i = z_i / d_i, \qquad i = 1 : n \tag{4b}$$

  - *Backward substitution:*

$$x_i = y_i - \sum_{k=i+1}^{\min(n,i+p)} l_{ki} x_k, \qquad i = n : -1 : 1 \tag{4c}$$

Tridiagonal Matrices

- **A** is tridiagonal ($p = q = 1$)
  - Equation (1a) becomes $k^* = \max(1, i-1, j-1)$
    - Only two nonzero entries per row or column $j = i, i+1$
  - *Factorization* (cf. (1)):

$$u_{ii} = a_{ii} - l_{i,i-1}u_{i-1,i} \tag{5a}$$

$$u_{i,i+1} = a_{i,i+1} \tag{5b}$$

$$l_{i+1,i} = a_{i+1,i}/u_{ii}, \qquad i = 1 : n \tag{5c}$$

    - Terms that do not exist (e.g., u_{01}, $l_{n+1,n}$) are zero
  - *Forward and backward substitution* (cf. (2)):

$$y_1 = b_1 \tag{6a}$$

$$y_i = b_i - l_{i,i-1}y_{i-1}, \qquad i = 2 : n \tag{6b}$$

$$x_n = y_n/u_{nn} \tag{6c}$$

$$x_i = \frac{1}{u_{ii}}(y_i - u_{i,i+1}y_{i+1}), \qquad i = n-1 : -1 : 1 \tag{6d}$$

- Implementing the tridiagonal procedure
  - Store the matrix by diagonals

$$l_i = a_{i,i-1}, \qquad a_i = a_{ii}, \qquad u_i = a_{i,i+1}$$

  - On output, replace l_i, a_i, u_i by their factors

The Tridiagonal Algorithm

```
function x = tridi(l, a, u, b)
% tridi: Solution of a tridiagonal system by Gaussian
% elimination. The vectorsl, a, u contain the subdiagonal,
% diagonal, and superdiagonal entries of an n-by-n
% tridiagonal matrix A. The solution of the system
% Ax = b is returned in x. The lower and upper
% triangular factors are stored as l and u.

   n = length(a);
%                          Factorization
   for i = 2:n
      l(i) = l(i)/a(i-1);
      a(i) = a(i) - l(i)*u(i-1);
   end
%                          Forward substitution
   x(1) = b(1);
   for i = 2:n
      x(i) = b(i) - l(i)*x(i-1);
   end
%                          Backward substitution
   x(n) = x(n)/a(n);
   for i = n-1: -1: 1
      x(i) = (x(i) - u(i+1)*x(i))/a(i)
   end
```

Pivoting with Banded Systems

- Pivoting alters the bandwidth
  - The upper bandwidth is enlarged
  - *Example 2.* Interchange the first two rows of the matrix of Example 1

$$\mathbf{A} = \begin{bmatrix} a_{21} & a_{22} & a_{23} & & & \\ a_{11} & a_{12} & & & & \\ a_{31} & a_{32} & a_{33} & a_{34} & & \\ & a_{42} & a_{43} & a_{44} & a_{45} & \\ & & a_{53} & a_{54} & a_{55} & a_{56} \\ & & & a_{64} & a_{65} & a_{66} \end{bmatrix}$$

    - The upper bandwidth is now $q = 2$
  - Some data structures cannot handle bandwidth changes
    - Others (to be discussed) can

Finite Difference Computation

- *Example 3.* A two-point boundary value problem

$$-w'' + w = 0, \qquad 0 < x < 1, \qquad w(0) = 0, \qquad w(1) = 1$$

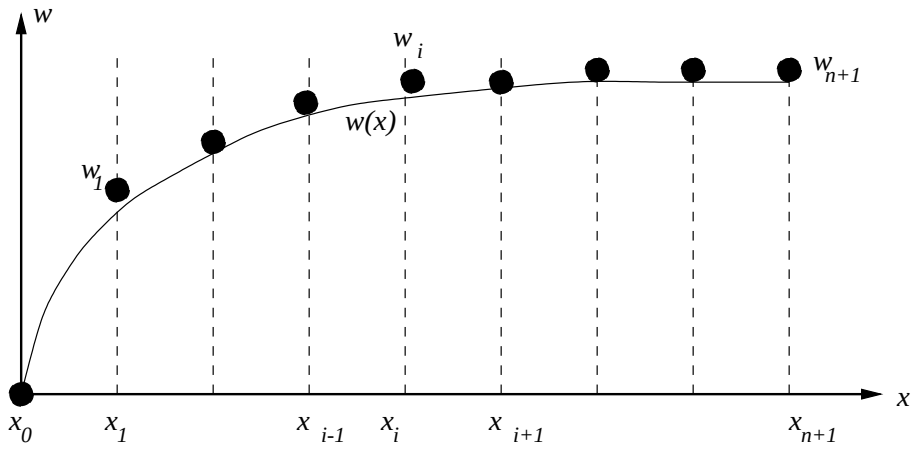
  - The exact solution is

$$w(x) = \frac{\sinh x}{\sinh 1}$$

- *Finite Difference Approximation:*

  - Introduce a mesh of spacing $h = 1/(n+1)$ on $[0, 1]$

    * Let $x_i = ih$, $i = 0 : n+1$



  - Approximate $w''(x_i)$ by central differences

$$w''(x_i) \approx \frac{w_{i-1} - 2w_i + w_{i+1}}{h^2}$$

    * w_i is the finite difference approximation of $w(x_i)$

  - Approximate the ODE at x_i

$$-\frac{w_{i-1} - 2w_i + w_{i+1}}{h^2} + w_i = 0$$

Finite Difference Computation

- Multiply by h^2

$$-w_{i-1} + (2 + h^2)w_i - w_{i+1} = 0$$

  - The discretization error is $O(h^2)$

- Use the difference equation at all interior mesh points

  - Use the boundary conditions $w_0 = 0$, $w_{n+1} = 1$

$$\begin{aligned}
(2 + h^2)w_1 - w_2 &= 0, \qquad && i = 1 \\
-w_{i-1} + (2 + h^2)w_i - w_{i+1} &= 0, \qquad && i = 2 : n - 1 \\
-w_n - 1 + (2 + h^2)w_n &= 1, \qquad && i = n
\end{aligned}$$

- The result is a tridiagonal linear system

$$\mathbf{Ax} = \mathbf{b}$$

  with

$$\mathbf{A} = \begin{bmatrix}
2 + h^2 & -1 & & & \\
-1 & 2 + h^2 & -1 & & \\
 & & \ddots & & \\
 & & -1 & 2 + h^2 & -1 \\
 & & & -1 & 2 + h^2
\end{bmatrix}$$

$$\mathbf{x} = [w_1,\ w_2,\ \cdots,\ w_n]^T, \qquad \mathbf{b} = [0,\ 0,\ \cdots,\ 1]^T$$

Finite Difference Computation

- The input to tridi is

$$\mathbf{a} = \begin{bmatrix} 2+h^2 \\ 2+h^2 \\ \vdots \\ 2+h^2 \end{bmatrix}, \qquad \mathbf{l} = \mathbf{u} = \begin{bmatrix} -1 \\ -1 \\ \vdots \\ -1 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

- Condition number of $\mathbf{A}$ as a function of n

n	h	$\kappa_2(\mathbf{A})$	$\kappa_2(\mathbf{A})h^2$
3	1/4	5.3629	0.3352
7	1/8	23.0147	0.3596
15	1/16	93.6675	0.3659
31	1/32	367.2897	0.3675
63	1/64	1506.8	0.3679
127	1/128	6028.7	0.3680

  - $\kappa_2(\mathbf{A}) = O(1/h^2)$
    - Accuracy and condition are at odds

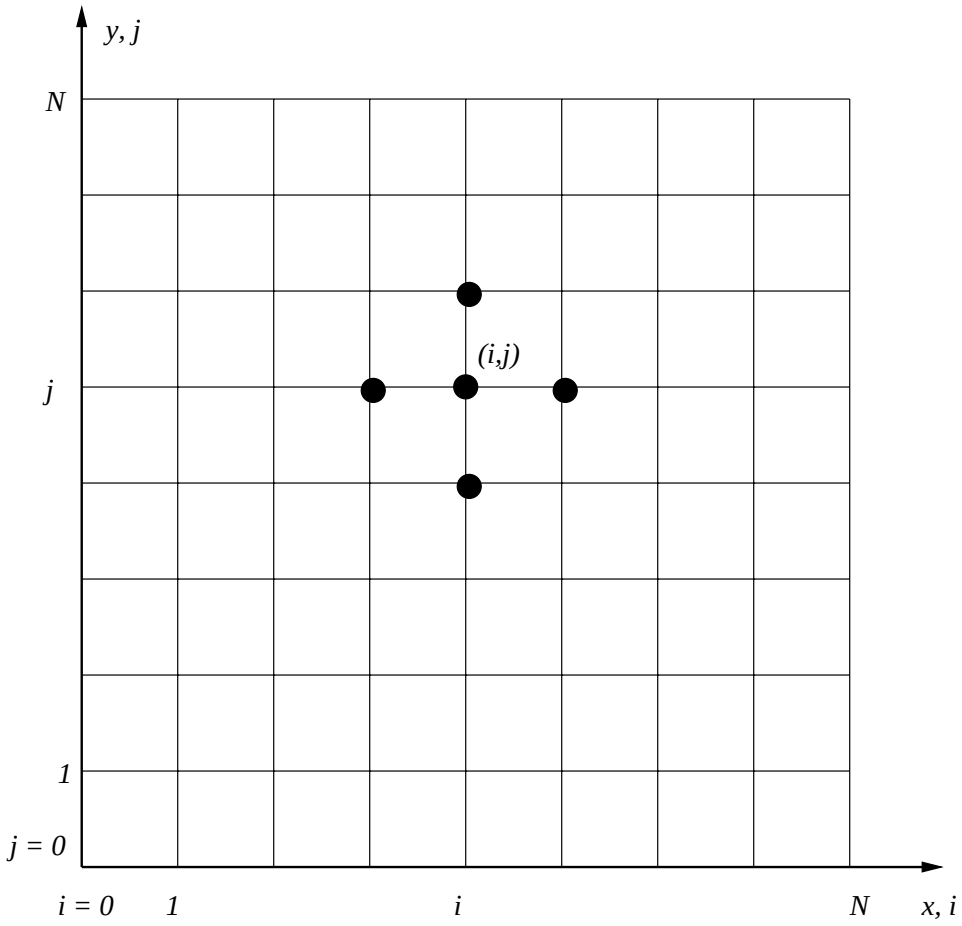
Two-Dimensional Finite Differences

- *Example 4.* Solving Poisson's equation on a square

$$-\Delta w := -w_{xx} - w_{yy} = f(x,y), \qquad (x,y) \in \Omega$$

$$w = g(x,y), \qquad (x,y) \in \partial\Omega$$

  - $\Omega = \{(x,y) | 0 < x, y < 1\}$
  - Divide Ω into N^2 squares of size $h \times h$ with $h = 1/N$
  - Let $x_i = ih$, $y_j = jh$



2D Finite Differences

- Approximate derivatives by central differences

$$w_{xx}(x_i, y_j) \approx \frac{w_{i-1,j} - 2w_{ij} + w_{i+1,j}}{h^2}$$

$$w_y y(x_i, y_j) \approx \frac{w_{i,j-1} - 2w_{ij} + w_{i,j+1}}{h^2}$$

  - w_{ij} is the finite difference approximation of $w(x_i, y_j)$
  - Approximate the PDE at (x_i, y_j)

$$-\frac{w_{i-1,j} - 2w_{ij} + w_{i+1,j}}{h^2} - \frac{w_{i,j-1} - 2w_{ij} + w_{i,j+1}}{h^2} = f(x_i, y_j)$$

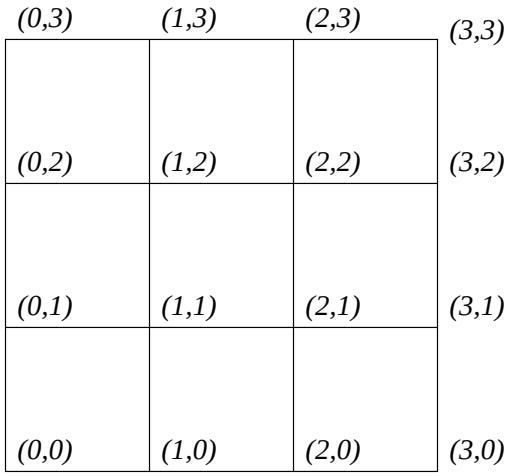
    or

$$-(w_{i-1,j} + w_{i+1,j} + w_{i,j-1} + w_{i,j+1}) + 4w_{ij} = h^2 f(x_i, y_j)$$

    * The difference equation at (x_i, y_j) connects w_{ij} to unknowns at its north, east, south, and west neighbors
    * The discretization error is $O(h^2)$

2D Finite Differences

- Use the difference equation at all interior nodes
  - Use the boundary conditions near edges and corners
    - For a 3×3 grid: write the difference equation at the points $(1,1)$, $(2,1)$, $(1,2)$, and $(2,2)$



$$4w_{11} - w_{21} - w_{12} = h^2 f_{11} + g_{01} + g_{10}$$
$$-w_{11} + 4w_{21} - w_{22} = h^2 f_{21} + g_{31} + g_{20}$$
$$-w_{11} + 4w_{12} - w_{22} = h^2 f_{12} + g_{02} + g_{13}$$
$$-w_{21} - w_{12} + 4w_{22} = h^2 f_{22} + g_{32} + g_{23}$$

    - $f_{ij} := f(x_i, y_j)$
    - The algebraic system is 4×4

- Order the equations and unknowns by rows

$$\begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{bmatrix} \begin{bmatrix} w_{11} \\ w_{21} \\ w_{12} \\ w_{22} \end{bmatrix} = \begin{bmatrix} h^2 f_{11} + g_{01} + g_{10} \\ h^2 f_{21} + g_{31} + g_{20} \\ h^2 f_{12} + g_{02} + g_{13} \\ h^2 f_{22} + g_{32} + g_{23} \end{bmatrix}$$

  - The structure of $\mathbf{A}$ is not apparent

2D Finite Differences

- The general finite difference system
  - Order the equations and unknowns by rows

$$\mathbf{x} = [\mathbf{x}_1^T,\ \mathbf{x}_2^T,\ \cdots,\ \mathbf{x}_{N-1}^T]^T \tag{7a}$$

    where

$$\mathbf{x}_j^T = [w_{1j},\ w_{2j},\ \cdots,\ 2_{N-1,j}] \tag{7b}$$

  - Write the difference equation at all interior nodes

$$\mathbf{A} = \begin{bmatrix}
4 & -1 & & & -1 & & & & & & & & & & \\
-1 & 4 & -1 & & & -1 & & & & & & & & & \\
 & & \ddots & & & & \ddots & & & & & & & & \\
 & & -1 & 4 & & & & -1 & & & & & & & \\
-1 & & & & 4 & -1 & & & -1 & & & & & & \\
 & -1 & & & -1 & 4 & -1 & & & -1 & & & & & \\
 & & \ddots & & & & \ddots & & & & \ddots & & & & \\
 & & & -1 & & & -1 & 4 & & & & -1 & & & \\
 & & & & & & & & & & & & & & \\
 & & & & & & & & & & \ddots & & & & \\
 & & & & & & & & & & & & & & \\
 & & & & & & & & -1 & & & & 4 & -1 & \\
 & & & & & & & & & -1 & & & -1 & 4 & -1 \\
 & & & & & & & & & & \ddots & & & & \ddots \\
 & & & & & & & & & & & -1 & & & -1 & 4
\end{bmatrix}$$

2D Finite Differences

- The algebraic system is *block tridiagonal*

$$\begin{bmatrix} \mathbf{C}_1 & \mathbf{D}_1 & & \\ \mathbf{D}_2 & \mathbf{C}_2 & \mathbf{D}_2 & \\ & & \ddots & \\ & & \mathbf{D}_{N-1} & \mathbf{C}_{N-1} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_{N-1} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_{N-1} \end{bmatrix} \tag{8a}$$

where

$$\mathbf{C}_j = \begin{bmatrix} 4 & -1 & & \\ -1 & 4 & -1 & \\ & & \ddots & \\ & & -1 & 4 \end{bmatrix}, \qquad \mathbf{D}_j = \begin{bmatrix} -1 & & & \\ & -1 & & \\ & & \ddots & \\ & & & -1 \end{bmatrix} \tag{8b}$$

and

$$\begin{aligned} \mathbf{b}_j = & h^2 \begin{bmatrix} f_{1j} \\ f_{2j} \\ \vdots \\ f_{N-1,j} \end{bmatrix} + \begin{bmatrix} g_{0j} \\ 0 \\ \vdots \\ 0 \\ g_{Nj} \end{bmatrix} - \delta_{1,j} \begin{bmatrix} g_{10} \\ g_{20} \\ \vdots \\ g_{N-1,0} \end{bmatrix} \\ & - \delta_{N-1,j} \begin{bmatrix} g_{1N} \\ g_{2N} \\ \vdots \\ g_{N-1,N} \end{bmatrix} \end{aligned} \tag{8c}$$

2D Finite Differences

- **Note:**

  i. Matrix Dimensions:
  - $\mathbf{C}_j$ is a $(N-1) \times (N-1)$ tridiagonal matrix
  - $\mathbf{D}_j$ is a $(N-1) \times (N-1)$ diagonal matrix
  - $\mathbf{A}$ is a $(N-1)^2 \times (N-1)^2$ block tridiagonal matrix

  ii. The Kronecker delta δ_{ij} is unity when $j = k$ and zero otherwise

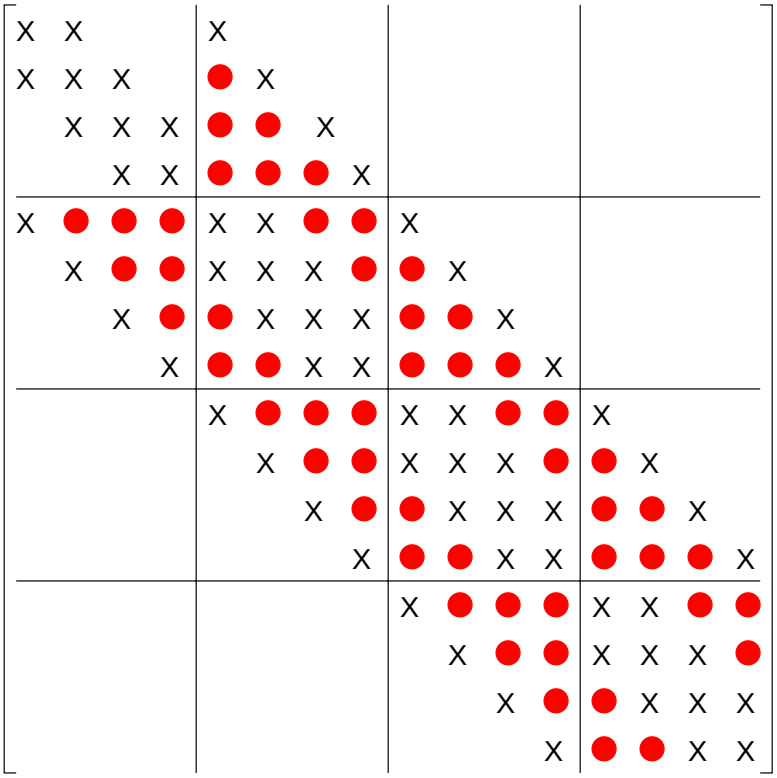
  iii. There are only 5 nonzero bands. The lower and upper bandwidths are $p = q = N - 1$

  iv. $\mathbf{D}_j$ is tridiagonal with finite element discretization
  - using a piecewise bilinear polynomial basis
  - The lower and upper bandwidths would be N

- *Fill In* for scalar band procedures
  - u_{ij} and l_{ij} involve inner products between the ith row of $\mathbf{L}$ and the jth column of $\mathbf{U}$
  - Zero elements within the band of $\mathbf{A}$ are nonzero in $\mathbf{L}$ and $\mathbf{U}$

Fill In

- Consider $N = 4$



X - *Original entry* ● - *Created by elimination*

  - **A** has about $5N^2$ nonzero entries
  - **L** and **U** require about $2N^3$ memory locations
  - With $n \approx N^2$ and $p = q \approx N$
    - Band factorization needs about N^4 multiplications
    - Full factorization needs about $N^6/3$ multiplications

Profile Schemes

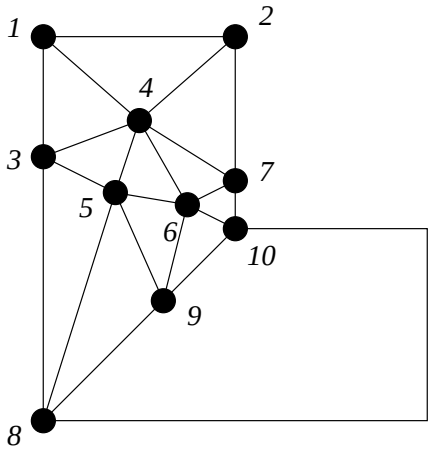
– Concentrate on symmetric positive definite systems

– There may be variations in the bandwidth

  * Due to pivoting
  * Due to nonuniform grids

– *Example 5.* Finite element matrix structure

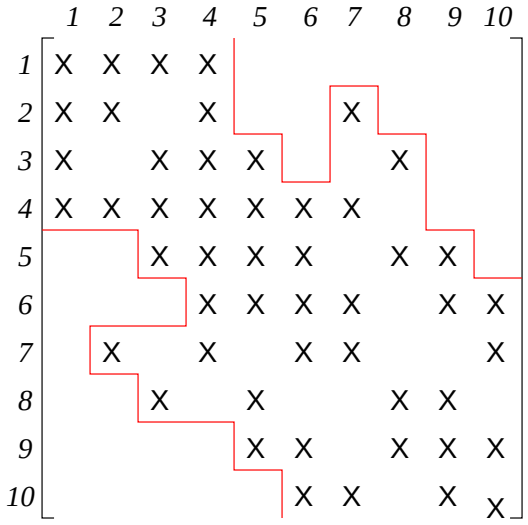
  * Unknowns at vertices are connected to unknowns on elements sharing the vertex
  * Equations and unknowns are ordered as shown



	1	2	3	4	5	6	7	8	9	10
1	X	X	X	X						
2	X	X		X			X			
3	X		X	X	X			X		
4	X	X	X	X	X	X	X			
5			X	X	X	X		X	X	
6				X	X	X	X		X	X
7		X		X		X	X			X
8			X		X			X	X	
9					X	X		X	X	X
10						X	X		X	X

Profile Schemes

- Account for local variation in bandwidth
  - The *skyline* or *profile* is the envelope formed by the local row or column bandwidths



  - **L** and **U** have the same profiles as **A**
  - Let m_i^* be the index of the first nonzero element of row i

$$l_{ij} = 0, \qquad 0 \le j < m_i^* \tag{9a}$$

and

$$k^* = \max(m_i^*, m_j^*) \tag{9b}$$

  - The profile form of the symmetric factorization (3) is

$$d_1 = a_{11} \tag{10a}$$

$$l_{ji} = \frac{1}{d_i}(a_{ji} - \sum_{k=k^*}^{i-1} d_k l_{jk} l_{ik}), \qquad i = m_j^* : j-1, \tag{10b}$$

$$d_j = a_{jj} - \sum_{k=m_j^*}^{j-1} d_k l_{jk}^2, \qquad j = 2 : n \tag{10c}$$

Profile Schemes

- The profile form of forward and backward substitution is

$$z_i = b_i - \sum_{k=m_i^*}^{i-1} l_{ik} z_k, \qquad i = 1 : n \tag{11a}$$

$$y_i = z_i / d_i, \qquad i = 1 : n \tag{11b}$$

$$x_i = y_i - \sum_{k=i+1}^{i+m_i^*} l_{ki} x_k, \qquad i = n : -1 : 1 \tag{11c}$$

  - Sums in (10, 11) are zero when a lower index exceeds an upper
  - $\mathbf{L}$ can be stored by rows (cf. Section 1.2)
    - Zeros within the profile become nonzero and are stored
  - The inner products in (10a,b) and (11a) involve row operations
    - All elements are within the profile
    - l_{ji} in (10b) is computed as u_{ij} and reflected
  - Backward substitution involves a column operation
    - Must test if an operation is inside the profile
    - Rewrite the operation using (row) saxpys

Profile Schemes

- *Example 6.* Column Identification

$$\mathbf{L} = \begin{bmatrix} \times & & & & & & & \\ \times & \times & & & & & & \\ \times & \times & \times & & & & & \\ \times & \times & \times & \times & & & & \\ & & & \times & \times & & & \\ & \times & \times & \times & \times & \times & & \\ & & & \times & \times & \times & \times & \\ & & \times & \times & \times & \times & \times & \times \end{bmatrix}$$

- The profile
  - The local (lower and upper) bandwidth of row i is $p_i = i - m_i^*$
  - The bandwidth of $\mathbf{A}$ is $p = \max_{1 \le i \le n} p_i$
  - The number of multiplications and divisions to factor $\mathbf{A}$ is

$$\Theta = \sum_{i=1}^{N-1} p_i(p_i + 3) \tag{12a}$$

  - The number of elements within the profile is

$$P = \sum_{i=1}^{N} p_i \tag{12b}$$

Profile Reduction

- Zero elements within the profile become nonzero during the factorization
  - Fill-in depends on the ordering of equations and unknowns
  - Methods for reducing bandwidth will reduce profile
    - Methods of reducing bandwidth are simpler
    - Methods for reducing profile are more effective
  - *Example 7.* Consider the 5×5 matrix

$$\mathbf{A} = \begin{bmatrix} \times & & & & \\ \times & \times & & & \\ \times & \bullet & \times & & \\ \times & \bullet & \bullet & \times & \\ \times & \bullet & \bullet & \bullet & \times \end{bmatrix} \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix}$$
$$\begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix}$$

    - $\mathbf{A}$ is symmetric but only the lower triangular portion is shown
    - All elements within the profile will fill in ($\bullet$)
    - Reversing the order of equations and unknowns produces a system with no fill in

$$\mathbf{A} = \begin{bmatrix} \times & & & & \\ & \times & & & \\ & & \times & & \\ & & & \times & \\ \times & \times & \times & \times & \times \end{bmatrix} \begin{matrix} 5 \\ 4 \\ 3 \\ 2 \\ 1 \end{matrix}$$
$$\begin{matrix} 5 & 4 & 3 & 2 & 1 \end{matrix}$$

Combat Graph Theory

- Reading: Saad (1996)
- A graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$ is defined by sets of vertices and edges

$$\mathcal{V} = \{v_1, v_2, \cdots, v_{N_v}\}, \qquad \mathcal{E} = \{e_1, e_2, \cdots, e_{N_e}\}$$

  with e_k consisting of pairs (v_i, v_j), $v_i, v_j \in \mathcal{V}$

- The *adjacency graph* representation of a symmetric matrix $\mathbf{A}$:

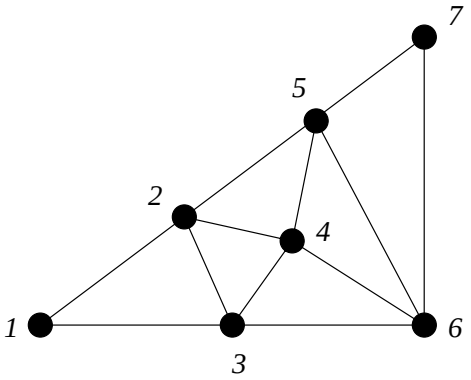
  i. Vertices of the graph correspond to rows of $\mathbf{A}$ (unknowns)

  ii. Edges of the graph correspond to nonzero elements of $\mathbf{A}$

  – Graph vertex i and j are connected if and only if $a_{ij} \neq 0$, $i \neq j$

- *Example 8.* The graph of a symmetric matrix $\mathbf{A}$ arising from a scalar PDE is often the mesh

$$\mathbf{A} = \begin{array}{c} \left[\begin{array}{ccccccc} \times & & & & & & \\ \times & \times & & & & & \\ \times & \times & \times & & & & \\ & \times & \times & \times & & & \\ & \times & & \times & \times & & \\ & & \times & \times & \times & \times & \\ & & & & \times & \times & \times \end{array}\right] \begin{array}{c} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \end{array} \\ \begin{array}{ccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 \end{array} \end{array}$$



Combat Graph Theory

- *Example 9.* Draw graphs of the matrices of Example 7

  - A symmetric permutation is equivalent to reordering the vertices of a graph
  - A symmetric permutation changes the rows and columns of a matrix so that the eigenvalues do not change

- The *degree of a vertex* of a graph is the number of edges incident on it

  - *Example 10.* The degree of Node 1 of Example 8 is 2, that of Node 4 is 4

- A *level set* consists of all unmarked neighbors of all nodes visited in a previous level set

Cuthill-McKee Algorithm

- Cuthill-McKee (CM) profile minimization technique:
  - Traverse a graph in level sets
  - Traverse the level set in order of increasing degree
  - Select the initial level set to consist of a single vertex v_1
    - Select v_1 on the periphery of $\mathcal{G}$

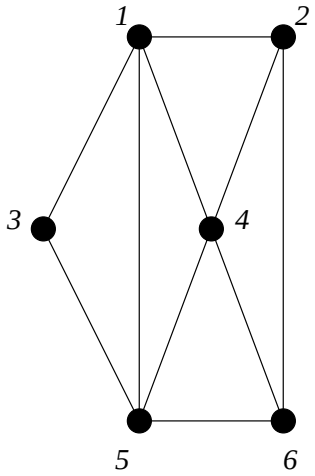
function $\mathcal{Q} = \mathrm{cm}(\mathcal{V})$
% cm: Cuthill-McKee procedure to number a set of vertices
% $\mathcal{V}$ to reduce the profile of a sparse matrix. The procedure
% begins with a starting vertex $v_1 \in \mathcal{V}$. On return, $\mathcal{Q}$
% stores the renumbered vertices.

$\mathcal{L} = \{v_1\}$;
$\mathcal{Q} = \mathcal{L}$;
while $\tilde{(}\mathcal{L} \in \emptyset)$
  For each vertex in $\mathcal{L}$ (in the order in which they are numbered)
    Append their unnumbered neighbors to $\mathcal{Q}$
    in order of increasing degree;
    $\mathcal{L} =$ { vertices just numbered };
  end
end

- This algorithm is slightly different than Saad's (1996)

Cuthill-McKee Algorithm

- *Example 11.* Consider the mesh shown

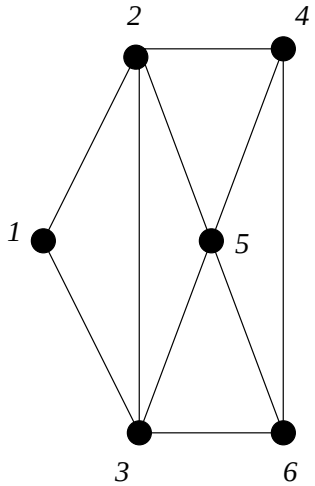


	1	2	3	4	5	6
1	X					
2	X	X				
3	X		X			
4	X	X		X		
5	X		X	X	X	
6		X		X	X	X

- Cuthill-McKee procedure with starting vertex 3

Level Set	Vertex	Neighbor	Degree	$\mathcal{Q}$
1	3	1	4	{3,
		5	4	1, 5,
2	1	2	3	
		4	4	2, 4,
	5	6	3	6}

- New numbering



	1	2	3	4	5	6
1	X					
2	X	X				
3	X	X	X			
4		X		X		
5		X	X	X	X	
6			X	X	X	X

Cuthill-McKee Algorithm

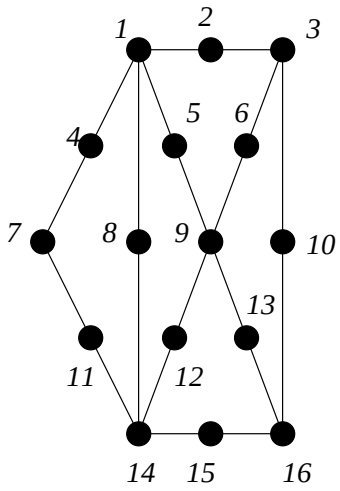
- *Example 12.* Consider the mesh and graph on the next page
  - Unknowns at midpoint nodes are only connected to those on elements containing the node
  - e.g., quadratic finite element approximation
- With row-by-row ordering: $p = 13$, $P = 106$
- First level set
  - Start at Node 7
    - $\mathcal{Q} = \{7\}$
  - Traverse the first level set

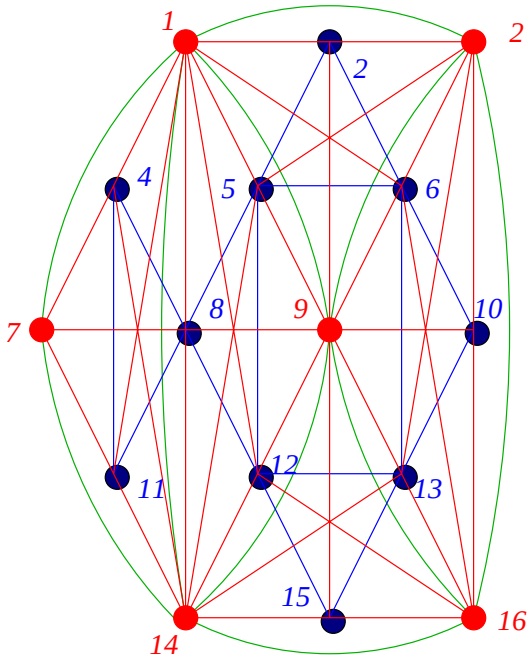
Vertex	Neighbors	Degree	$\mathcal{Q}$
7	1	11	$\{7,$
	4	5	
	8	8	
	11	5	
	14	11	4, 11, 8, 1, 14$\}$

  - After the first level-set traversal:

$$\mathcal{L} = \{4,\ 11,\ 8,\ 1,\ 14\}, \qquad \mathcal{Q} = \{7,\ 4,\ 11,\ 8,\ 1,\ 14\}$$

Example 12: Row-by-Row Order





	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	X															
2	X	X														
3	X	X	X													
4	X			X												
5	X	X	X		X											
6	X	X	X		X	X										
7	X			X			X									
8	X			X	X		X	X								
9	X	X	X		X	X		X	X							
10			X			X			X	X						
11	X			X			X	X			X					
12	X				X			X	X			X				
13			X			X			X	X		X	X			
14	X			X	X		X	X	X		X	X	X	X		
15									X			X	X	X	X	
16			X			X			X	X		X	X	X	X	X

Example 12: Cuthill-McKee Order

- Level Set 2:

$$\mathcal{L} = \{4,\ 11,\ 8,\ 1,\ 14\}, \qquad \mathcal{Q} = \{7,\ 4,\ 11,\ 8,\ 1,\ 14\}$$

Vertex	Neighbors	Degee
4		
11		
8	5	8
	9	12
	12	8
1	2	5
	3	8
	6	8
14	13	8
	15	5
	16	8

  - The new order

$$\mathcal{L} = \{5,\ 12,\ 9,\ 2,\ 3,\ 6,\ 15,\ 13\}$$

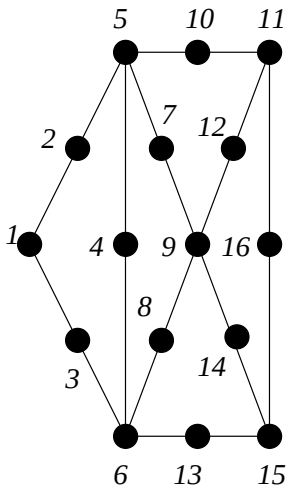
$$\mathcal{Q} = \{7,\ 4,\ 11,\ 8,\ 1,\ 14,\ 5,\ 12,\ 9,\ 2,\ 3,\ 6,\ 15,\ 13,\ 16\}$$

- Third level set: The only unnumbered vertex is 10

$$\mathcal{Q} = \{7,\ 4,\ 11,\ 8,\ 1,\ 14,\ 5,\ 12,\ 9,\ 2,\ 3,\ 6,\ 15,\ 13,\ 16,\ 10\}$$

Example 12: Cuthill-McKee Order

- Bandwidth and profile: $p = 9$, $P = 76$



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	X															
2	X	X														
3	X	X	X													
4	X	X	X	X												
5	X	X	X	X	X											
6	X	X	X	X	X	X										
7				X	X	X	X									
8				X	X	X	X	X								
9				X	X	X	X	X	X							
10					X		X		X	X						
11					X		X		X	X	X					
12					X		X		X	X	X	X				
13						X		X	X				X			
14						X		X	X		X	X	X	X		
15						X		X	X		X	X	X	X	X	
16									X		X	X		X	X	X

eeKcM-llihtuC Algorithm

- George (1971) [1] reversed the numbering given by the Cuthill-McKee algorithm
  - This is called the *Reverse Cuthill-McKee (RCM)* algorithm
  - George proves that the profile of RCM is never larger than that of CM
- The RCM ordering for Example 12 is

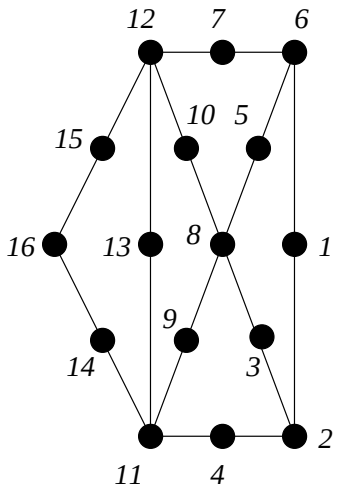
  $$\{10,\ 16,\ 13,\ 15,\ 6,\ 3,\ 2,\ 9,\ 12,\ 5,\ 14,\ 1,\ 8,\ 11,\ 4,\ 7\}$$

- The MATLAB procedure *symrcm* performs RCM on symmetric matrics
  - It produced the same ordering as above with 12 and 5 interchanged and 4 and 7 interchanged
  - Evidently, 4 was the starting node
  - This gave the same profile as the above ordering
- The MATLAB procedure *spy* will plot the nonzero structure of a sparse matrix

[1] J.A. George (1971), "Computer Implementation of the Finite Element Method," Rep. STAN-CS-71-208, Dept. Comp. Sci., Stanford University, Palo Alto

Example 12: RCM Oder

- Bandwidth and profile: $p = 9$, $P = 68$

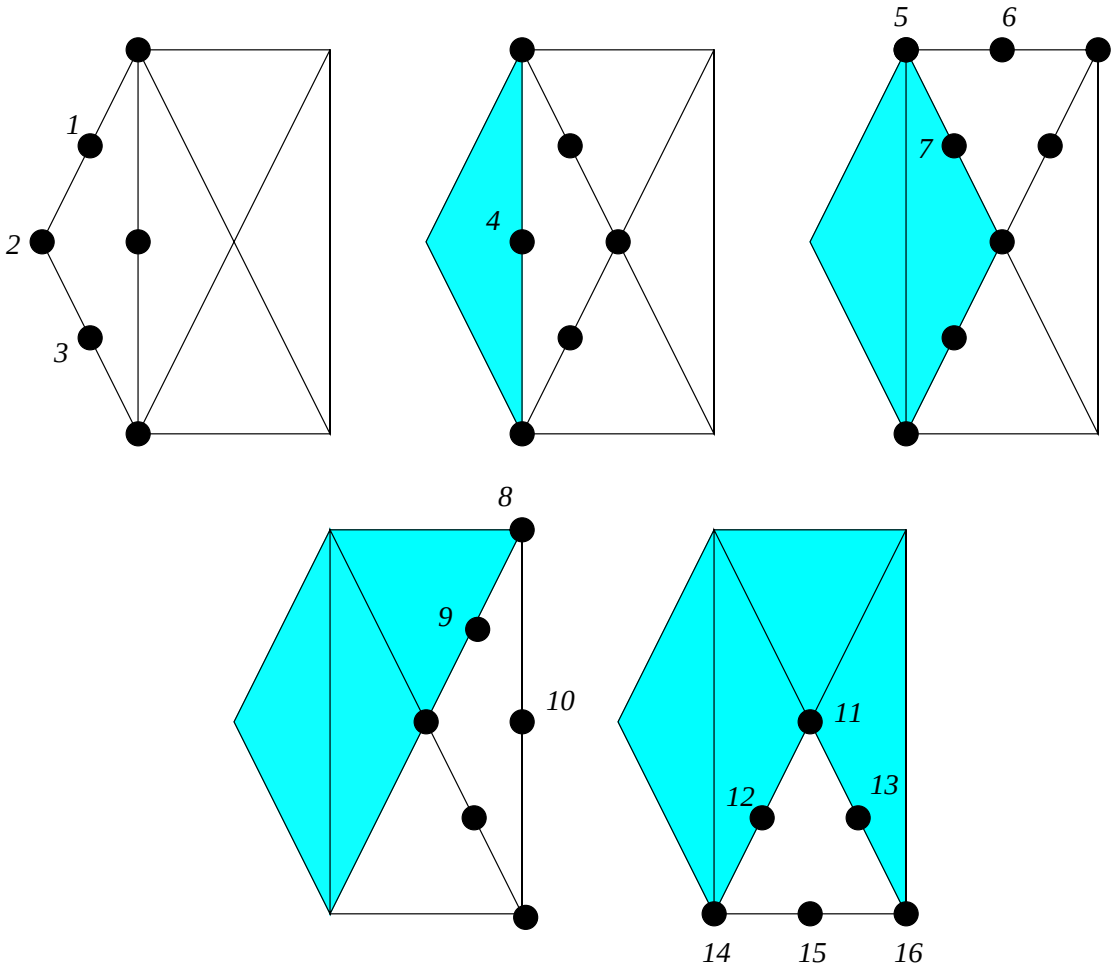


	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	X															
2	X	X														
3	X	X	X													
4		X	X	X												
5	X	X	X		X											
6	X	X	X		X	X										
7					X	X	X									
8	X	X	X	X	X	X	X	X								
9		X	X	X				X	X							
10					X	X	X	X	X	X						
11		X	X	X				X	X	X	X					
12					X	X	X	X	X	X	X	X				
13								X	X	X	X	X	X			
14											X	X	X	X		
15											X	X	X	X	X	
16											X	X	X	X	X	X

Wave-Front Ordering

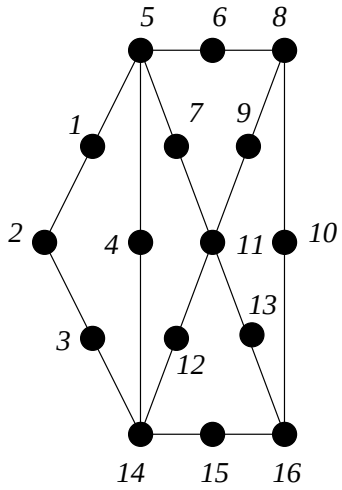
- "Frontal" or "wave front" techniques:
  - Select unknowns x_i that only depend on themselves
    - They form the initial level set
    - If none, select an unknown on the periphery of the graph
  - All unknowns that only involve those in Level Set 1 form Level Set 2
  - All unknowns that only involve those in Level Sets 1 and 2 form Level Set 3, etc.
- For finite element problems, this can be regarded as element annihilation
  - cf. J.A. George and J.W. Liu (1981)
- *Example 13.* Consider the problem of Example 12
  - Select an element and number the unknowns that are not connected to unknowns on other elements
  - Remove the element
  - Proceed to an adjacent element and repeat the process

Wave-Front Ordering



Wave-Front Ordering

- Wave-Front bandwidth and profile: $p = 13$, $P = 68$



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	X															
2	X	X														
3	X	X	X													
4	X	X	X	X												
5	X	X	X	X	X											
6					X	X										
7				X	X	X	X									
8					X	X	X	X								
9					X	X	X	X	X							
10								X	X	X						
11				X	X	X	X	X	X	X	X					
12				X	X		X				X	X				
13								X	X	X	X	X	X			
14	X	X	X	X	X		X				X	X	X	X		
15											X	X	X	X	X	
16								X	X	X	X	X	X	X	X	X

3.3. Block Tridiagonal Systems

- Example 2.4 produced the block tridiagonal system of the form

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1a}$$

or

$$\begin{bmatrix} \mathbf{A}_1 & \mathbf{B}_1 & & \\ \mathbf{C}_2 & \mathbf{A}_2 & \mathbf{B}_2 & \\ & & \ddots & \\ & & \mathbf{C}_n & \mathbf{A}_n \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_n \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_n \end{bmatrix} \tag{1b}$$

  - $\mathbf{A}_k$, $\mathbf{C}_k$, $\mathbf{B}_k$, $k = 1 : n$, are $q \times q$
  - The blocks of Example 2.4 were symmetric

$$\mathbf{A}_j = \begin{bmatrix} 4 & -1 & & \\ -1 & 4 & -1 & \\ & & \ddots & \\ & & -1 & 4 \end{bmatrix}$$

$$\mathbf{B}_j = \mathbf{C}_j = \begin{bmatrix} -1 & & & \\ & -1 & & \\ & & \ddots & \\ & & & -1 \end{bmatrix}$$

  - Do not assume symmetry ($\mathbf{B}_j \neq \mathbf{C}_j + 1$)
    - But do not pivot (dangerous)

The Block Tridiagonal algorithm

- Assume a factorization of the form

$$\mathbf{L} = \begin{bmatrix} \mathbf{I} & & & \\ \mathbf{L}_2 & \mathbf{I} & & \\ & \ddots & & \\ & & \mathbf{L}_n & \mathbf{I} \end{bmatrix}, \qquad \mathbf{U} = \begin{bmatrix} \mathbf{U}_1 & \mathbf{B}_1 & & \\ & \mathbf{U}_2 & \mathbf{B}_2 & \\ & & \ddots & \\ & & & \mathbf{U}_n \end{bmatrix} \tag{2}$$

  - Multiply

$$\mathbf{U}_1 = \mathbf{A}_1 \tag{3a}$$

$$\mathbf{L}_i \mathbf{U}_{i-1} = \mathbf{C}_i, \qquad i = 2 : n \tag{3b}$$

$$\mathbf{L}_i \mathbf{B}_{i-1} + \mathbf{U}_i = \mathbf{A}_i, \qquad i = 2 : n \tag{3c}$$

- Factorization

  $\mathbf{U}_1 = \mathbf{A}_1$;
  for i = 2:n
    Factor $\mathbf{U}_{i-1}^T$ and determine the rows of $\mathbf{L}_i$ from
      $\mathbf{U}_{i-1}^T \mathbf{L}_i^T = \mathbf{C}_i^T$ by forward and backward
      substitution;
    $\mathbf{U}_i = \mathbf{A}_i - \mathbf{L}_i \mathbf{b}_{i-1}$;
  end

- Forward and backward substitution: from (1, 2)

$$\mathbf{y}_1 = \mathbf{b}_1 \tag{4a}$$

$$\mathbf{y}_i = \mathbf{b}_i - \mathbf{L}_i \mathbf{y}_{i-1}, \qquad i = 2 : n \tag{4b}$$

$$\mathbf{U}_n \mathbf{x}_n = \mathbf{y}_n \tag{4c}$$

$$\mathbf{U}_i \mathbf{x}_i = \mathbf{y}_i - \mathbf{b}_i \mathbf{x}_{i+1}, \qquad i = n-1 : -1 : 1 \tag{4d}$$

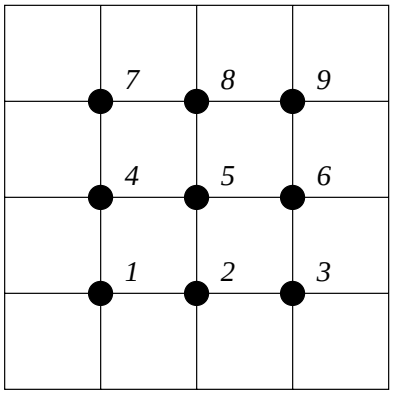
  - Save $\mathbf{U}_i$ in factored form from (3b)

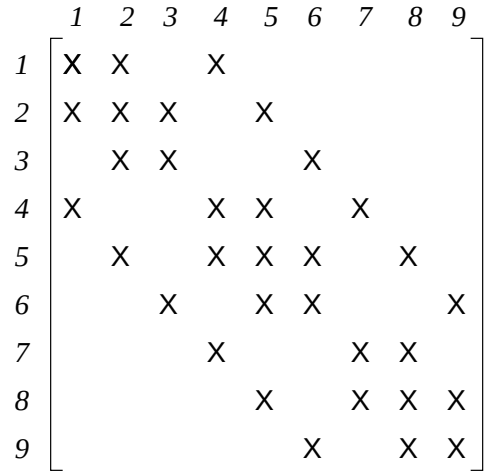
The Tridiagonal Algorithm

- Operation count
  - $2q^3/3$ FLOPs to factor $\mathbf{U}_{i-1}$ in (3b)
  - $2q^3$ FLOPs to determine $\mathbf{L}_i$ in (3b)
  - $2q^3$ FLOPs to determine $\mathbf{U}_i$ in (3c)
  - Summing on i, we have $14nq^3/3$ multiplications to factor
  - The forward and backward substitution takes $O(nq^2)$ FLOPs
  - $\mathbf{U}_i$ and $\mathbf{L}_i$ are not tridiagonal even if $\mathbf{A}_i$ is
- Band vs Block
  - Depends on the sizes of p (the bandwidth) and q (the block size)
  - For the 2D Poisson equation on an $N \times N$ grid (Example 2.4), $p \approx q$
    - Banded factorization has approximately $2N^4$ FLOPs
    - Block factorization has $n \approx N^2$ and $q \approx N$ for approximately $14N^5/3$ FLOPs
    - Some reductions in the block operation count are possible by accounting for the sparsity of $\mathbf{B}_i$ and $\mathbf{C}_i$

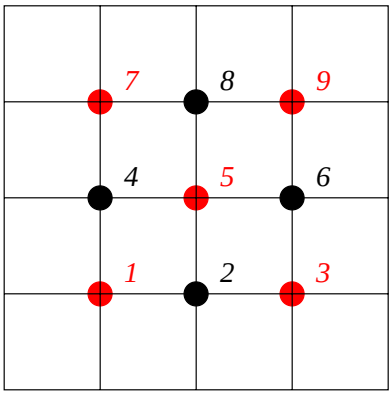
Two-Dimensional Poisson Equation

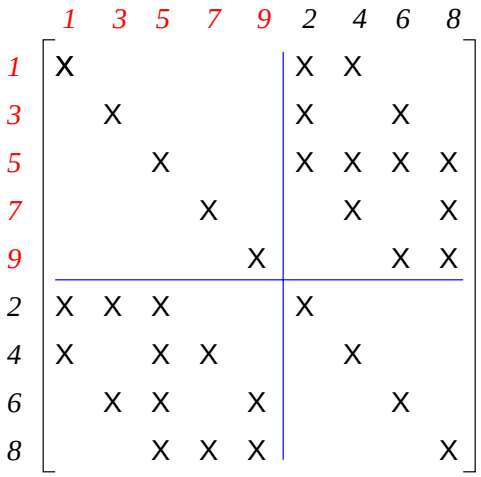
- *Example 1.* Consider Poisson's equation on an $N \times N$ grid (cf. Example 2.4)
  - Finite differencing for a 4×4 problem
  - Row-by-row numbering with a single index





- Write equations at the odd points first
  - Order the odd unknowns first





Odd-Even Ordering

- The structure of the matrix with odd-even ordering is

$$\mathbf{A} = \begin{bmatrix} \mathbf{D}_1 & \mathbf{V}_1 \\ \mathbf{V}_2 & \mathbf{D}_2 \end{bmatrix}$$

- To solve

$$\begin{bmatrix} \mathbf{D}_1 & \mathbf{V}_1 \\ \mathbf{V}_2 & \mathbf{D}_2 \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{bmatrix}$$

  - Factor

$$\begin{bmatrix} \mathbf{D}_1 & \mathbf{V}_1 \\ \mathbf{V}_2 & \mathbf{D}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{L}_2 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{U}_1 & \mathbf{B}_1 \\ \mathbf{0} & \mathbf{U}_2 \end{bmatrix}$$

  - Expand the factorization

$$\mathbf{U}_1 = \mathbf{D}_1, \qquad \mathbf{B}_1 = \mathbf{V}_1$$

$$\mathbf{L}_2 = \mathbf{V}_2\mathbf{U}_1^{-1}, \qquad \mathbf{U}_2 = \mathbf{D}_2 - \mathbf{L}_2\mathbf{V}_1$$

  - Forward and backward substitution

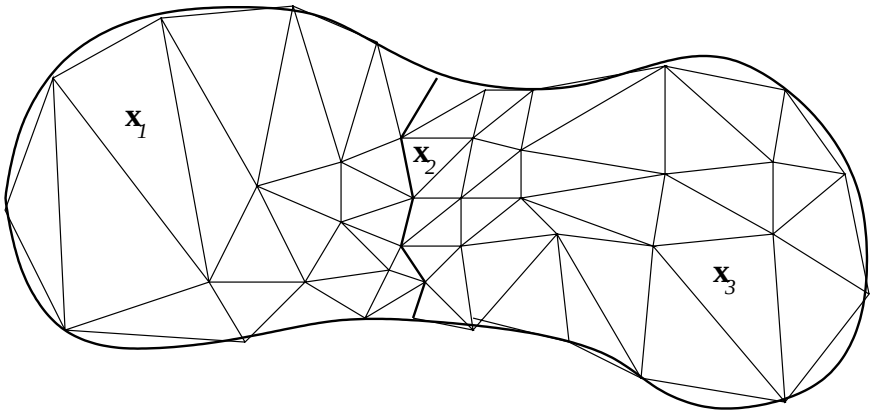
$$\mathbf{y}_1 = \mathbf{b}_1, \qquad \mathbf{y}_2 = \mathbf{b}_2 - \mathbf{V}_2\mathbf{U}_1^{-1}\mathbf{y}_1$$

$$\mathbf{U}_2\mathbf{x}_2 = \mathbf{y}_2, \qquad \mathbf{D}_1\mathbf{x}_1 = \mathbf{y}_1 - \mathbf{V}_1\mathbf{x}_2$$

  - $\mathbf{U}_2$ is penta-diagonal

Domain Decomposition

- "Dissection," "substructuring," and "domain decomposition"
  - Partition $\mathbf{A}$ into three pieces so that
    - The unknowns $\mathbf{x}_1$ are only connected to $\mathbf{x}_3$
    - The unknowns $\mathbf{x}_2$ are only connected to $\mathbf{x}_3$
  - Occurs "naturally" in finite difference and finite element applications



  - The structure of the system is

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{0} & \mathbf{A}_{13} \\ \mathbf{0} & \mathbf{A}_{22} & \mathbf{A}_{23} \\ \mathbf{A}_{13}^T & \mathbf{A}_{23}^T & \mathbf{A}_{33} \end{bmatrix} \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{bmatrix} \qquad (5)$$

- Suppose $\mathbf{A}$ is symmetric
  - Factor $\mathbf{A}$ into $\mathbf{L}\mathbf{D}\mathbf{L}^T$

$$\mathbf{L} = \begin{bmatrix} \mathbf{I} & & \\ & \mathbf{I} & \\ \boldsymbol{\omega}_{13}^T & \boldsymbol{\omega}_{23}^T & \mathbf{I} \end{bmatrix}, \qquad \mathbf{D} = \begin{bmatrix} \mathbf{D}_1 & & \\ & \mathbf{D}_2 & \\ & & \mathbf{D}_3 \end{bmatrix}$$

Domain Decomposition

- Factorization procedure

  function $[\mathbf{L}, \mathbf{D}] = \mathrm{dd}(\mathbf{A})$
  % dd: block factorization of a matrix $\mathbf{A}$ into $\mathbf{LDL}^T$

  for k = 1:2
    $\mathbf{D}_k = \mathbf{A}_{kk}$;
    Solve $\mathbf{D}_k \boldsymbol{\omega}_{k3} = \mathbf{A}_{k3}$ for $\boldsymbol{\omega}_{k3}$;
  end
  $\mathbf{D}_3 = \mathbf{A}_{33} - \boldsymbol{\omega}_{13}^T \mathbf{D}_1 \boldsymbol{\omega}_{13} - \boldsymbol{\omega}_{23}^T \mathbf{D}_2 \boldsymbol{\omega}_{23}$;

- **Note:**

  i. $\mathbf{D}_1$ and $\mathbf{D}_2$ can be factored without knowledge of each other or $\mathbf{D}_3$, $\boldsymbol{\omega}_{13}$, and $\boldsymbol{\omega}_2 3$

  ii. The factorizations of $\mathbf{D}_1$ and $\mathbf{D}_2$ can be done in parallel

  iii. Design modifications only change those matrices affected

  iv. The procedure can be done recursively

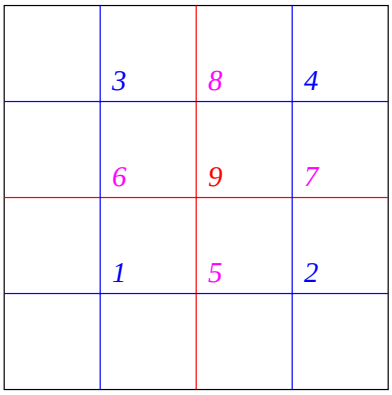
  v. $\mathbf{D}_3$ is called the *Schur complement* of $\mathbf{A}$

  - For $N \times N$ grid problems, George (1973) [1] shows that factorization takes $O(N^3)$ FLOPs
  - Banded and profile techniques require $O(N^4)$ FLOPs
  - Nested dissection has the optimal order of operations

[1] J.A. George (1973), Nested dissection of a regular finite element mesh, *SIAM J. Numer. Anal.*, **10**, 345-363

Nested Dissection

- Two-dimensional nested dissection
  - Bisect the domain
  - Number unknowns on the fine level first
  - Number unknowns on the interface between two regions next
  - Number unknowns at the juncture of four regions last
- Nested ordering of a 4×4 mesh



	1	2	3	4	5	6	7	8	9
1	X				X	X			
2		X			X		X		
3			X			X		X	
4				X			X	X	
5	X	X			X				X
6	X		X			X			X
7		X		X			X		X
8			X	X				X	X
9					X	X	X	X	X

4. Orthogonalization and Least Squares
4.1. Orthogonality and the Singular Value Decomposition

- Reading Trefethen and Bau (1997), Lecture 2
- *Orthogonal vectors:*
  - Orthogonal bases are better conditioned than others
- **Definition 1:** $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\} \in \Re^m$ is *orthogonal* if

$$\mathbf{x}_i^T \mathbf{x}_j = 0, \qquad i \neq j \tag{1a}$$

  - The vectors are *orthonormal* if

$$\mathbf{x}_i^T \mathbf{x}_j = \delta_{ij}, \qquad i \neq j \tag{1b}$$

- **Definition 2:** Two subspaces $\mathcal{S}_1, \mathcal{S}_2 \in \Re^m$ are orthogonal if $\mathbf{x}^T\mathbf{y} = 0$ for all $\mathbf{x} \in \mathcal{S}_1$ and all $\mathbf{y} \in \mathcal{S}_2$
  - $\mathcal{S}_2$ is called the *orthogonal complement* of $\mathcal{S}_1$
- **Theorem 1:** If $\mathbf{A} \in \Re^{m\times n}$ then range($\mathbf{A}$) is the orthogonal complement of null($\mathbf{A}^T$)
  - *Proof:* Let $\mathbf{y} \in$ range($\mathbf{A}$) and $\mathbf{x} \in$ null($\mathbf{A}^T$)
  - With $\mathbf{z} \in \Re^n$, let $\mathbf{y} = \mathbf{Az}$

$$\mathbf{y}^T\mathbf{x} = (\mathbf{Az})^\mathbf{T}\mathbf{x} = \mathbf{z}^\mathbf{T}\mathbf{A}^\mathbf{T}\mathbf{x} = \mathbf{z}^\mathbf{T}(\mathbf{A}^\mathbf{T}\mathbf{x}) = \mathbf{0}$$

  - Because $\mathbf{A}^T\mathbf{x} = 0$ $\square$

Orthogonality

- **Definition 3:** Vectors $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_k\}$ form an *orthonormal basis* for a subspace $\mathcal{S} \in \Re^m$ if they are orthonormal and span $\mathcal{S}$
- **Definition 4:** A matrix $\mathbf{Q} \in \Re^{m \times m}$ is *orthogonal* if

$$\mathbf{Q}^T\mathbf{Q} = \mathbf{I} \tag{2}$$

  - Thus, $\mathbf{Q}^{-1} = \mathbf{Q}^T$
  - The columns of $\mathbf{Q}$ form an orthonormal basis for $\Re^m$
- $||\ ||_2$ is invariant under orthogonal transformations
  - If $\mathbf{Q}$ is orthogonal

$$||\mathbf{Qx}||_2^2 = \mathbf{x}^T\mathbf{Q}^T\mathbf{Qx} = \mathbf{x}^T\mathbf{x} = ||\mathbf{x}||_2^2$$

- The matrix 2 and F norms are also invariant under orthogonal transformations
  - If $\mathbf{Q}$ and $\mathbf{z}$ are orthogonal

$$||\mathbf{QAZ}||_\mathbf{2} = ||\mathbf{A}||_\mathbf{2}, \qquad ||\mathbf{QAZ}||_\mathbf{F} = ||\mathbf{A}||_\mathbf{F} \tag{3}$$

    * The proof follows that for a vector norm

The Singular Value Decomposition

- Reading: Trefethen and Bau (1997), Lectures 4 and 5
- **Theorem 2 (Singular Value Decomposition (SVD):)** Let $\mathbf{A} \in \Re^{m \times n}$, then there exists orthogonal matrices $\mathbf{U} \in \Re^{m \times m}$ and $\mathbf{V} \in \Re^{n \times n}$ such that

$$\mathbf{U}^T \mathbf{A} \mathbf{V} = \mathbf{\Sigma} \tag{4a}$$

  - $\mathbf{\Sigma} \in \Re^{m \times n}$

$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_p \\ & & & \\ & & & \end{bmatrix} \tag{4b}$$

  - $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_p$, $p = min(m, n)$

- *Proof:* Let

$$\mathbf{A}\mathbf{x} = \sigma \mathbf{y}, \qquad ||\mathbf{x}||_2 = ||\mathbf{y}||_2 = 1, \qquad ||\mathbf{A}||_2 = \sigma \tag{5}$$

  - Define orthogonal matrices $\mathbf{U}$ and $\mathbf{V}$ such that

$$\mathbf{U} = [\mathbf{y}, \mathbf{u}_2, \cdots, \mathbf{u}_m] = [\mathbf{y}, \mathbf{U}_1]$$

$$\mathbf{V} = [\mathbf{x}, \mathbf{v}_2, \cdots, \mathbf{v}_n] = [\mathbf{x}, \mathbf{V}_1]$$

    * Any orthonormal set of vectors can be extended to form an orthonormal basis

SVD

– Construct

$$\mathbf{U}^T\mathbf{A}\mathbf{V} = \begin{bmatrix} \mathbf{y}^T \\ \mathbf{U}_1^T \end{bmatrix} \mathbf{A} \begin{bmatrix} \mathbf{x} & \mathbf{V}_1 \end{bmatrix} = \begin{bmatrix} \mathbf{y}^T\mathbf{A}\mathbf{x} & \mathbf{y}^T\mathbf{A}\mathbf{V}_1 \\ \mathbf{U}_1^T\mathbf{A}\mathbf{x} & \mathbf{U}_1^T\mathbf{A}\mathbf{V}_1 \end{bmatrix}$$

– Use (5)

* $\mathbf{y}^T\mathbf{A}\mathbf{x} = \sigma$
* $\mathbf{U}_1^T\mathbf{A}\mathbf{x} = \sigma\mathbf{U}_1^T\mathbf{y} = 0$

– Thus

$$\mathbf{U}^T\mathbf{A}\mathbf{V} = \begin{bmatrix} \sigma & \mathbf{y}^T\mathbf{A}\mathbf{V}_1 \\ \mathbf{0} & \mathbf{U}_1^T\mathbf{A}\mathbf{V}_1 \end{bmatrix} := \begin{bmatrix} \sigma & \mathbf{w}^T \\ \mathbf{0} & \mathbf{B} \end{bmatrix} := \mathbf{A_1}$$

– Select $\mathbf{z}^T = [\sigma, \mathbf{w}^T]$ and compute

$$\mathbf{A}_1\mathbf{z} = \begin{bmatrix} \sigma & \mathbf{w}^T \\ \mathbf{0} & \mathbf{B} \end{bmatrix} \begin{bmatrix} \sigma \\ \mathbf{w} \end{bmatrix} = \begin{bmatrix} \sigma^2 + \mathbf{w}^T\mathbf{w} \\ \mathbf{B}\mathbf{w} \end{bmatrix}$$

– Then

$$||\mathbf{A}_1\mathbf{z}||_2^2 = (\sigma^2 + \mathbf{w}^T\mathbf{w})^2 + \mathbf{w}^T\mathbf{B}^T\mathbf{B}\mathbf{w} \geq (\sigma^2 + \mathbf{w}^T\mathbf{w})^2$$

– Thus,

$$||\mathbf{A}_1||_2^2 \geq \frac{||\mathbf{A}_1\mathbf{z}||_2^2}{||\mathbf{z}||_2^2} \geq \sigma^2 + \mathbf{w}^T\mathbf{w}$$

SVD

– Since $\mathbf{U}$ and $\mathbf{V}$ are orthogonal, use (3) to obtain

$$\sigma^2 = ||\mathbf{A}||_2^2 = ||\mathbf{U}^T\mathbf{A}\mathbf{V}||_2^2 = ||\mathbf{A}_1||_2^2$$

– Thus, $\mathbf{w} = 0$

– An induction argument completes the proof □

- $\sigma_1, \sigma_2, \cdots, \sigma_p$ are the *singular values* of $\mathbf{A}$
  - Let $\mathbf{u}_i$ and $\mathbf{v}_i$ be the $i\ th$ columns of $\mathbf{U}$ and $\mathbf{V}$
    - $\mathbf{u}_i$ and $\mathbf{v}_i$ are the left and right *singular vectors*
    - The singular vectors satisfy

$$\mathbf{A}\mathbf{v}_i = \sigma_i\mathbf{u}_i, \qquad \mathbf{A}\mathbf{u}_i = \sigma_i\mathbf{v}_i, \qquad i = 1:p \tag{6}$$

- Some properties of singular values
  - If $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > \sigma_{r+1} = \cdots = \sigma_p = 0$, then

$$\text{rank}(\mathbf{A}) = r \tag{7a}$$

$$\text{null}(\mathbf{A}) = \text{span}\{\mathbf{v}_{r+1}, \mathbf{v}_{r+2}, \cdots, \mathbf{v}_n\} \tag{7b}$$

$$\text{range}(\mathbf{A}) = \text{span}\{\mathbf{u}_1, \mathbf{u}_2, \cdots, \mathbf{u}_r\} \tag{7c}$$

$$\mathbf{A} = \sum_{i=1}^{r} \sigma_i\mathbf{u}_i\mathbf{v}_i^T \tag{7d}$$

$$||\mathbf{A}||_F^2 = \sigma_1^2 + \sigma_2^2 + \cdots + \sigma_p^2, \qquad p = \min(m,n) \tag{7e}$$

$$||\mathbf{A}||_2 = \sigma_1 \tag{7f}$$

Orthogonal Projections

- Reading: Trefethen and Bau (1997), Lecture 6
- **Definition 5:** $\mathbf{P} \in \Re^{n \times n}$ is the *orthogonal projection* onto a subspace $\mathcal{S} \subset \Re^{n \times n}$ if

$$\text{range}(\mathbf{P}) = \mathcal{S}, \qquad \mathbf{P}^2 = \mathbf{P}, \qquad \mathbf{P}^T = \mathbf{P} \tag{8}$$

  - If $\mathbf{x} \in \Re^n$ and $\mathbf{P}\mathbf{x} \in \mathcal{S}$ then $(\mathbf{I} - \mathbf{P})\mathbf{x}$ is in the orthogonal complement of $\mathcal{S}$
  - The orthogonal projection onto a subspace is unique
- Let the columns of $\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k]$ form an orthonormal basis for a subspace $\mathcal{S}$
  - $\mathbf{P} = \mathbf{V}\mathbf{V}^T$ is the unique orthogonal projection onto $\mathcal{S}$
    - $\mathbf{V}\mathbf{V}^T$ is symmetric
    - $\mathbf{P}^2 = \mathbf{V}\mathbf{V}^T\mathbf{V}\mathbf{V}^T = \mathbf{V}\mathbf{V}^T$ by orthogonality
    - If $\mathbf{x} \in \Re^n$ then $\mathbf{y} = \mathbf{P}\mathbf{x} = \mathbf{V}(\mathbf{V}^T\mathbf{x})$
    - $\mathcal{S} = \text{span}\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_k\}$, $\text{range}(\mathbf{P}) = \mathcal{S}$

Orthogonal Projections

- Some Properties:
  - Let rank($\mathbf{A}$) = r and partition $\mathbf{U}$ and $\mathbf{V}$

$$\mathbf{U} = [\mathbf{U}_r, \mathbf{U}_{m-r}], \qquad \mathbf{V} = [\mathbf{V}_r, \mathbf{V}_{n-r}] \tag{9}$$

    - $\mathbf{U}_r \in \Re^{m \times r}$, $\mathbf{U}_{m-r} \in \Re^{m \times (m-r)}$
    - $\mathbf{V}_r \in \Re^{n \times r}$, $\mathbf{V}_{n-r} \in \Re^{n \times (n-r)}$
  - $\mathbf{U}_r \mathbf{U}_r^T$ is a projection onto range($\mathbf{A}$)
  - $\mathbf{U}_{m-r} \mathbf{U}_{m-r}^T$ is a projection onto null($\mathbf{A}^T$)
    - the orthogonal complement of range($\mathbf{A}$)
  - $\mathbf{V}_r \mathbf{V}_r^T$ is a projection onto range($\mathbf{A}^T$)
    - the orthogonal complement of null($\mathbf{A}$)
  - $\mathbf{V}_{n-r} \mathbf{V}_{n-r}^T$ is a projection onto null($\mathbf{A}$)

Orthogonal Projections

- *Example 1.* The singular value decomposition of

$$\mathbf{A} = \begin{bmatrix} 2 & 1 & 3 \\ 1 & 0 & 5 \\ 3 & 1 & 8 \end{bmatrix}$$

is

$$\mathbf{U} = \begin{bmatrix} 0.3393 & -0.7427 & -0.5774 \\ 0.4735 & 0.6652 & -0.5774 \\ 0.8128 & -0.0775 & 0.5774 \end{bmatrix}$$

$$\mathbf{\Sigma} = \begin{bmatrix} 10.5826 & 0 & 0 \\ 0 & 1.4174 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{V} = \begin{bmatrix} 0.3393 & -0.7427 & 0.5774 \\ 0.1089 & -0.5786 & -0.8083 \\ 0.9344 & 0.3371 & -0.1155 \end{bmatrix}$$

- With $\sigma_3 = 0$ we have $r = 2$
- Verify that $\mathbf{U}^T\mathbf{U} = \mathbf{I}$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}$

Orthogonal Projections

- Partition $\mathbf{U}$ and $\mathbf{V}$

$$\mathbf{U}_r = \begin{bmatrix} 0.3393 & -0.7427 \\ 0.4735 & 0.6652 \\ 0.8128 & -0.0775 \end{bmatrix}, \qquad \mathbf{U}_{m-r} = \begin{bmatrix} -0.5774 \\ -0.5774 \\ 0.5774 \end{bmatrix}$$

$$\mathbf{V}_r = \begin{bmatrix} 0.3393 & -0.7427 \\ 0.1089 & -0.5786 \\ 0.9344 & 0.3371 \end{bmatrix}, \qquad \mathbf{V}_{n-r} = \begin{bmatrix} 0.5774 \\ -0.8083 \\ -0.1155 \end{bmatrix}$$

- The projections

$$\mathbf{U}_r\mathbf{U}_r^T = \begin{bmatrix} 0.6667 & -0.3333 & 0.3333 \\ -0.3333 & 0.6667 & 0.3333 \\ 0.3333 & 0.3333 & 0.6667 \end{bmatrix}$$

$$\mathbf{U}_{m-r}\mathbf{U}_{m-r}^T = \begin{bmatrix} 0.3333 & 0.3333 & -0.3333 \\ 0.3333 & 0.3333 & -0.3333 \\ -0.3333 & -0.3333 & 0.3333 \end{bmatrix}$$

$$\mathbf{V}_r\mathbf{V}_r^T = \begin{bmatrix} 0.6667 & 0.4667 & 0.0667 \\ 0.4667 & 0.3467 & -0.0933 \\ 0.0667 & -0.0933 & 0.9867 \end{bmatrix}$$

$$\mathbf{V}_{n-r}\mathbf{V}_{n-r}^T = \begin{bmatrix} 0.3333 & -0.4667 & -0.0667 \\ -0.4667 & 0.6533 & 0.0933 \\ -0.0667 & 0.0933 & 0.0133 \end{bmatrix}$$

Orthogonal Projections

- Verify that $\mathbf{U}_r^T\mathbf{U}_r = \mathbf{I}$, etc
- Verify that
  - $\mathbf{U}_r\mathbf{U}_r^T + \mathbf{U}_{n-r}\mathbf{U}_{n-r}^T = \mathbf{I}$
  - $\mathbf{V}_r\mathbf{V}_r^T + \mathbf{V}_{n-r}\mathbf{V}_{n-r}^T = \mathbf{I}$
- Choose $\mathbf{x} = [1, 0, 0]^T$ and calculate

$$\mathbf{y} = \mathbf{V}_{n-r}\mathbf{V}_{n-r}^T\mathbf{x} = \begin{bmatrix} 0.3333 \\ -0.4667 \\ -0.0667 \end{bmatrix}$$

  - Verify that $\mathbf{A}\mathbf{y} = 0$
  - Verify that $\mathbf{A}\mathbf{V}_{n-r}\mathbf{V}_{n-r}^T = \mathbf{0}$
- Similarly, verify that $\mathbf{A}^T\mathbf{U}_{m-r}\mathbf{U}_{m-r}^T = \mathbf{0}$

4.2. Rotations and Reflections

- Reading: Trefethen and Bau (1997), Lecture 10
- *Example 1.* Consider

$$\mathbf{Q} = \begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

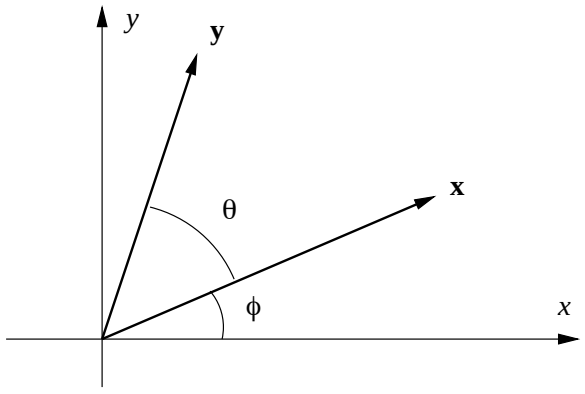
  - $\mathbf{Q}$ is orthogonal since $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$
  - $\mathbf{y} = \mathbf{Q}^T\mathbf{x}$ is a rotation of $\mathbf{x}$ through θ degrees
    - Let

$$\mathbf{x} = ||\mathbf{x}||_2[\cos\phi,\ \sin\phi]^T$$

    - Multiply

$$\begin{aligned} \mathbf{y} &= ||\mathbf{x}||_2 \begin{bmatrix} \cos\theta & -\sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\ &= ||\mathbf{x}||_2 \begin{bmatrix} \cos(\theta+\phi) \\ \sin(\theta+\phi) \end{bmatrix} \end{aligned}$$

  - $\mathbf{Q}$ is called a *rotation*



Reflections

- *Example 2.* Consider

$$\mathbf{Q} = \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix}$$

  - $\mathbf{Q}$ is orthogonal since $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$
  - $\mathbf{y} = \mathbf{Q}^T\mathbf{x} = \mathbf{Q}\mathbf{x}$ is a reflection of $\mathbf{x}$ across the line

$$\mathbf{z} = C[\cos\theta/2,\ \sin\theta/2]^T$$

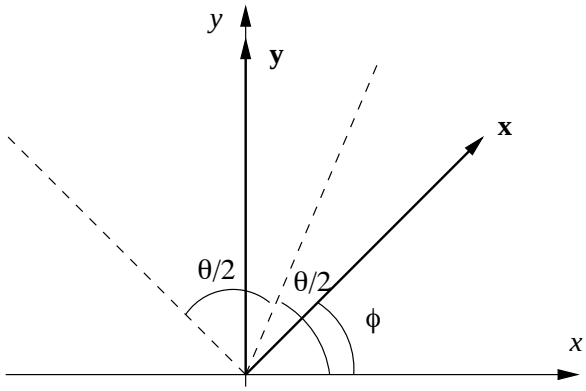
    * Let

$$\mathbf{x} = ||\mathbf{x}||_2[\cos\phi,\ \sin\phi]^T$$

    * Multiply

$$\begin{aligned} \mathbf{y} &= ||\mathbf{x}||_2 \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi \\ \sin\phi \end{bmatrix} \\ &= ||\mathbf{x}||_2 \begin{bmatrix} \cos(\theta-\phi) \\ \sin(\theta-\phi) \end{bmatrix} \end{aligned}$$

  - $\mathbf{Q}$ is called a *reflection*



Householder Reflections

- **Definition 1:** A *reflection* $\mathbf{P} \in \Re^{n \times n}$ has the form

$$\mathbf{P} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}, \qquad \mathbf{v} \in \Re^n \tag{1}$$

  - Also called a
    - Plane reflection
    - Householder reflection
    - Householder matrix

- Some Properties of Householder Matrices:
- $p_{ij} = \delta_{ij} - 2v_iv_j/(\mathbf{v}^T\mathbf{v})$, δ_{ij} is the Kronecker delta
- $\mathbf{P}$ is symmetric
- $\mathbf{P}$ is orthogonal

$$\mathbf{P}^T\mathbf{P} = \mathbf{P}^2 = (\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}})$$

$$= \mathbf{I} - 4\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} + 4\frac{\mathbf{v}(\mathbf{v}^T\mathbf{v})\mathbf{v}^T}{(\mathbf{v}^T\mathbf{v})^2} = \mathbf{I}$$

  - Thus, $\mathbf{P} = \mathbf{P}^T = \mathbf{P}^-1$

- $\mathbf{P}$ is a rank-1 modification of $\mathbf{I}$

Reflections

- $\mathbf{P}$ can be constructed annihilate components of a vector
  - Given $\mathbf{x}$, construct $\mathbf{P}$ such that $\mathbf{Px} = c\mathbf{e}_1$
  - Consider

$$\mathbf{Px} = \left(\mathbf{I} - 2\frac{\mathbf{vv}^T}{\mathbf{v}^T\mathbf{v}}\right)\mathbf{x} = \mathbf{x} - 2\frac{\mathbf{v}^T\mathbf{x}}{\mathbf{v}^T\mathbf{v}}\mathbf{v}$$

  - Select $\mathbf{v} = \mathbf{x} + \alpha\mathbf{e}_1$

$$\mathbf{v}^T\mathbf{x} = \mathbf{x}^T\mathbf{x} + \alpha x_1$$

$$\mathbf{v}^T\mathbf{v} = \mathbf{x}^T\mathbf{x} + 2\alpha x_1 + \alpha^2$$

  - Thus,

$$\mathbf{Px} = \mathbf{x} - 2\frac{\mathbf{x}^T\mathbf{x} + \alpha x_1}{\mathbf{x}^T\mathbf{x} + 2\alpha x_1 + \alpha^2}(\mathbf{x} + \alpha\mathbf{e}_1)$$

  - For $\mathbf{Px}$ to be in the direction of $\mathbf{e}_1$ we want

$$1 - 2\frac{\mathbf{x}^T\mathbf{x} + \alpha x_1}{\mathbf{x}^T\mathbf{x} + 2\alpha x_1 + \alpha^2} = \frac{\alpha^2 - \mathbf{x}^T\mathbf{x}}{\mathbf{x}^T\mathbf{x} + 2\alpha x_1 + \alpha^2} = \mathbf{0}$$

  - Thus, $\alpha = \pm||\mathbf{x}||_2$

Reflections

- In summary, selecting

$$\mathbf{v} = \mathbf{x} \pm ||\mathbf{x}||_2 \mathbf{e}_1 \tag{2a}$$

  Makes

$$\mathbf{P}\mathbf{x} = -2\alpha \frac{\mathbf{x}^T\mathbf{x} + \alpha x_1}{\mathbf{x}^T\mathbf{x} + 2\alpha x_1 + \alpha^2}\mathbf{e}_1 = -(\pm||\mathbf{x}||_2)\mathbf{e}_1 \tag{2b}$$

- What's this $\pm$ thing?
  - If $\mathbf{x}$ is nearly parallel to $\mathbf{e}_1$ then

$$\mathbf{v} = \mathbf{x} - ||\mathbf{x}||_2 \mathbf{e}_1$$

    has a small norm which could magnify roundoff errors
  - To minimize this, choose

$$\mathbf{v} = \mathbf{x} + \text{sign}(x_1)||\mathbf{x}||_2 \mathbf{e}_1 \tag{2c}$$

- A program for Householder vectors

```
function v = house(x)
% house: Compute the Householder vector v that
% annihilates all but the first component of x.

  n = length(x)
  v = x;
  v(1) = x(1) + sign(x(1))*norm (x);
```

Reflections

- *Example 3* (cf. Golub and Van Loan (1993), Problem 5.1.1). Let $\mathbf{x} = [1,\ 7,\ 2,\ 3,\ -1]^T$. Find $\mathbf{P}$
  - $||\mathbf{x}||_2 = 8$
  - $\mathbf{v} = [9,\ 7,\ 2,\ 3,\ -1]^T$
  - The reflection is

$$\mathbf{P} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}} = \mathbf{I} - \frac{1}{72}\begin{bmatrix} 81 & 63 & 18 & 27 & -9 \\ 63 & 49 & 14 & 21 & -7 \\ 18 & 14 & 4 & 6 & -2 \\ 27 & 21 & 6 & 9 & -3 \\ -9 & -7 & -2 & -3 & 1 \end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} -0.1250 & -0.8750 & -0.2500 & -0.3750 & 0.1250 \\ -0.8750 & 0.3194 & -0.1944 & -0.2917 & 0.0972 \\ -0.2500 & -0.1944 & 0.9444 & -0.0833 & 0.0278 \\ -0.3750 & -0.2917 & -0.0833 & 0.8750 & 0.0417 \\ 0.1250 & 0.0972 & 0.0278 & 0.0417 & 0.9861 \end{bmatrix}$$

  - The result is $\mathbf{P}\mathbf{x} = [-8,\ 0,\ 0,\ 0,\ 0]^T$

Reflections

- $\mathbf{P}$ never needs explicit generation and storage
  - Application of $\mathbf{P}$ to an $n \times n$ matrix $\mathbf{A}$ would require $O(n^3)$ FLOPs
  - Compute

$$\mathbf{PA} = \left(\mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}\right)\mathbf{A} = \mathbf{A} + \mathbf{v}\mathbf{w}^T \tag{3a}$$

    where

$$\mathbf{w} = \beta\mathbf{A}^T\mathbf{v}, \qquad \beta = -2/\mathbf{v}^T\mathbf{v} \tag{3b}$$

    * This requires $O(n^2)$ operations

- Function for a pre-Householder update

```
function A = row.house(A, v)
% row.house: Overwrite A ∈ ℜ^{m×n} with the product
% PA where P = I − 2vv^T/(v^Tv) is a Householder
% matrix and v is an m-vector.

β = −2/(v^T ∗ v);
w = β ∗ A^T ∗ v;
A = A + v ∗ w^T;
```

Reflections

- Function for a post-Householder update

  function $\mathbf{A} = \text{col.house}(\mathbf{A}, \mathbf{v})$
  % col.house: Overwrite $\mathbf{A} \in \Re^{m \times n}$ with the product
  % $\mathbf{AP}$ where $\mathbf{P} = \mathbf{I} - 2\mathbf{v}\mathbf{v}^T/(\mathbf{v}^T\mathbf{v})$ is a Householder
  % matrix and $\mathbf{v}$ is an n-vector.

  $\beta = -2/(\mathbf{v}^T * \mathbf{v})$;
  $\mathbf{w} = \beta * \mathbf{A} * \mathbf{v}$;
  $\mathbf{A} = \mathbf{A} + \mathbf{w} * \mathbf{v}^T$;

- *Example 4.* Let $\mathbf{A} \in \Re^{m \times n}$. Compute $\mathbf{Q}$ such that $\mathbf{B} = \mathbf{QA}$ has $b_{kj} = 0$, $k = j + 1 : m$
  - Partition $\mathbf{A}$

    $$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix}$$

    * where $\mathbf{A}_{11} \in \Re^{(j-1)\times(j-1)}$, $\mathbf{A}_{12} \in \Re^{(j-1)\times(n-j)}$, $\mathbf{A}_{21} \in \Re^{(m-j)\times(j-1)}$, and $\mathbf{A}_{22} \in \Re^{(m-j)\times(n-j)}$
  - Let

    $$\mathbf{Q} = \begin{bmatrix} \mathbf{I}_{j-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{P} \end{bmatrix} = \mathbf{I} - 2\frac{\mathbf{v}\mathbf{v}^T}{\mathbf{v}^T\mathbf{v}}, \qquad \mathbf{v} = \begin{bmatrix} \mathbf{0} \\ \tilde{\mathbf{v}} \end{bmatrix}$$

Reflections

- Multiply

$$\mathbf{B} = \mathbf{QA} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{PA}_{21} & \mathbf{PA}_{22} \end{bmatrix}$$

- A typical case is to apply the transform to each column with a goal of making $\mathbf{B}$ upper triangular
  - In this case, $\mathbf{A}_{21} = \mathbf{0}$
- The following code segment does the job

$\mathbf{v}(j:m) = \text{house}(\mathbf{A}(j:m, j));$
$\mathbf{A}(j:m, j, n) = \text{row.house}(\mathbf{A}(j:m, j:n), \mathbf{v}(j:m));$
$\mathbf{A}(j+1:m, j) = \mathbf{v}(j+1:m);$

  - The first line creates the nonzero portion of $\mathbf{v}$ that zeros b_{kj}, $k = j+1:m$
  - The second line applies the transformation $\mathbf{Q}$ to $\mathbf{A}_{22}$ and stores the result back in $\mathbf{A}$
  - The third line stores the nonzero portion of $\mathbf{v}$ in the zeroed portion of the $j\ th$ column of $\mathbf{A}$

Reflections

- Householder transformations are often applied in sequence

$$\mathbf{Q} = \mathbf{Q}_1 \mathbf{Q}_2 \cdots \mathbf{Q}_r$$

  where

$$\mathbf{Q}_j = \mathbf{I} - 2\frac{\mathbf{v}^{(j)}\left(\mathbf{v}^{(j)}\right)^T}{\left(\mathbf{v}^{(j)}\right)^T \mathbf{v}^{(j)}}, \qquad \mathbf{v}^{(j)} = \begin{bmatrix} \mathbf{0} \\ \tilde{\mathbf{v}}^{(j)} \end{bmatrix}$$

  - The dimension $\tilde{\mathbf{v}}^{(j)}$ is $m - j + 1$

- It is typically not necessary to store $\mathbf{Q}$, but rather store the Householder vectors $\mathbf{v}^{(j)}$, $j = 1 : r$
  - Suppose $\mathbf{v}^{(j)}$ is stored in the lower triangular part of a matrix $\mathbf{A}$
  - The following code segment overwrites $\mathbf{C}$ with $\mathbf{QC}$

```
for j = 1 : r
    v(j+1 : n) = A(j+1 : n, j);
    v(j) = 1;
    C(j : n, 1 : n) = row.house(C(j : n, j : n), v(j : n));
end
```

  - This can be done in $O(n^2 r)$ operations.
    - Direct computation of $\mathbf{Q}$ requires $O(n^3)$ operations

Rotations

- **Definition 2:** A *rotation* $\mathbf{G}(i,j,\theta) \in \Re^{n\times n}$ has the form

$$\mathbf{G}(i,j,\theta) = \begin{bmatrix} 1 & & 0 & & 0 & & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & & \vdots \\ 0 & & 0 & & 0 & & 1 \end{bmatrix} \begin{matrix} \\ \\ i \\ \\ j \\ \\ \\ \end{matrix} \qquad (4a)$$

$$\begin{matrix} & & i & & j & & \end{matrix}$$

$$c = \cos\theta, \qquad s = \sin\theta \qquad (4b)$$

  - The transformation is called a
    - plane rotation
    - Givens rotation

- Some Properties of Givens Rotations
  - $\mathbf{G}(i,j,\theta)$ is orthogonal
  - $\mathbf{G}(i,j,\theta)$ is a rank-2 modification of $\mathbf{I}$
  - The multiplication $\mathbf{G}(i,j,\theta)^T\mathbf{x}$ is a counterclockwise rotation of $\mathbf{x}$ in the i,j plane

Rotations

- If $\mathbf{x} \in \Re^n$ then

$$\mathbf{y} = \mathbf{G}(i,j,\theta)^T\mathbf{x}, \qquad y_k = \begin{cases} cx_i - sx_j, & \text{if } k = i \\ sx_i + cx_j, & \text{if } k = j \\ x_k, & \text{otherwise} \end{cases} \tag{5a}$$

- If we want $y_j = 0$ then

$$c = \frac{x_i}{\sqrt{x_i^2 + x_j^2}}, \qquad s = \frac{-x_j}{\sqrt{x_i^2 + x_j^2}} \tag{5b}$$

- Calculation of a Givens rotation

```
function [c, s] = givens(a, b)
% givens: Compute the Givens transformation c, s such
% that ca - sb = r and sa + cb = 0.

  if b = 0
     c = 1;
     s = 0;
  elseif | b | > | a |
     tau = -a/b;
     s = 1/ sqrt(1 + tau^2);
     c = s*tau;
  else
     tau = -b/a;
     c = 1/ sqrt(1 + tau^2);
     s = c*tau;
  end
```

Rotations

- Function for a pre-Givens rotation
  - The multiplication only affects rows i and j
  - Regard $\mathbf{A}$ as a $2 \times q$ matrix and compute

$$\mathbf{B} = \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \mathbf{A}$$

    - $\mathbf{B}$ is $2 \times q$
  - Overwrite $\mathbf{B}$ with $\mathbf{A}$

```
function A = row.rot(A, c, s)
% row.rot: Compute the rotation G(i,j,θ)A where
% A ∈ ℜ^{2×q}. The rotation is stored in A.

   [m, q] = size(A);
   for k = 1:q
      tau = A(1,k);
      sigma = A(2,k);
      A(1,k) = c*tau - s*sigma;
      A(2,k) = s*tau + c*sigma;
   end
```

Rotations

- Function for a post-Givens rotation
  - The multiplication only affects columns i and j

function $\mathbf{A}$ = col.rot($\mathbf{A}$, c, s)
% col.rot: Compute the rotation $\mathbf{A}\mathbf{G}^T(i, j, \theta)$ where
% $\mathbf{A} \in \Re^{q \times 2}$. The rotation is stored in $\mathbf{A}$.

```
[m,q] = size(A);
for k = 1:q
   tau = A(k,1);
   sigma = A(k,2);
   A(k,1) = c*tau - s*sigma;
   A(k,2) = s*tau + c*sigma;
end
```

- Each algorithm requires $4q$ multiplications and $2q$ additions
- Let $\mathbf{A} \in \Re^{m \times n}$ be such that $a_{kl} = 0$ $k = i-1 : i$, $l = 1 : j-1$
  - To make $a_{ij} = 0$ by rotating rows $i-1$ and i

```
[c,s] = givens(A(i-1,j), A(i,j))
A (i-1:i,j:n) = row.rot(A (i-1:i,j:n), c, s)
```

Rotations

- *Example 5.* Set $a_{33} = 0$ by a rotation of rows 2 and 3 when

$$\mathbf{A} = \begin{bmatrix} 3 & 2 & 6 & 7 \\ 0 & 0 & 5 & 1 \\ 0 & 0 & 12 & -3 \end{bmatrix}$$

  - Using the function [c, s] = givens(5,12) yields

$$c = -0.3846, \qquad s = 0.9231$$

    * Observe that $c^2 + s^2 = 1$

  - Performing $\mathbf{A}$ (2:3, 3:4) = row.rot ($\mathbf{A}$(2:3, 3:4), c, s) yields

$$\mathbf{A} = \begin{bmatrix} 3 & 2 & 6 & 7 \\ 0 & 0 & -13 & 2.3846 \\ 0 & 0 & 0 & 2.0769 \end{bmatrix}$$

4.3. The QR Reduction

- Reading Trefethen and Bau (1997), Lecture 7
- The **QR** factorization of a matrix $\mathbf{A} \in \Re^{m \times n}$ is

$$\mathbf{A} = \mathbf{QR} \tag{1}$$

  - $\mathbf{Q} \in \Re^{m \times m}$ is an orthogonal matrix
  - $\mathbf{R} \in \Re^{m \times n}$ is upper triangular
  - Assume (for the moment) $m \geq n$
- *Motivation:*
  - An alternate to Gaussian elimination when solving

$$\mathbf{Ax} = \mathbf{b}$$

    - More expensive than Gaussian elimination
  - Determining bases for orthogonal subspaces
  - Determining numerical rank through the SVD
  - Solving least squares problems

$$\min_{\mathbf{x}} ||\mathbf{Ax} - \mathbf{b}||_2$$

  - Solving algebraic eigenvalue problems

$$\mathbf{Ax} = \lambda \mathbf{x}$$

Householder QR Factorization

- Use Householder reflections to reduce successive columns of $\mathbf{A}$ to zero below their main diagonals
  - Suppose $m = 6$, $n = 4$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \\ a_{51} & a_{52} & a_{53} & a_{54} \\ a_{61} & a_{62} & a_{63} & a_{64} \end{bmatrix}$$

  - Construct a reflection $\mathbf{H}_1$ such that

$$\mathbf{H}_1\mathbf{A} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & a_{24}^{(1)} \\ 0 & a_{32}^{(1)} & a_{33}^{(1)} & a_{34}^{(1)} \\ 0 & a_{42}^{(1)} & a_{43}^{(1)} & a_{44}^{(1)} \\ 0 & a_{52}^{(1)} & a_{53}^{(1)} & a_{54}^{(1)} \\ 0 & a_{62}^{(1)} & a_{63}^{(1)} & a_{64}^{(1)} \end{bmatrix}$$

Householder QR Factorization

- Use a reflection to annihilate $a_{i2}^{(1)}$, $i = 3:6$

$$\mathbf{P}_2 \begin{bmatrix} a_{22}^{(1)} \\ a_{32}^{(1)} \\ a_{42}^{(1)} \\ a_{52}^{(1)} \\ a_{62}^{(1)} \end{bmatrix} = \begin{bmatrix} r_{22} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

  - Apply the transformation

$$\mathbf{H}_2 = \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & \mathbf{P}_2 \end{bmatrix}$$

    to get

$$\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ 0 & r_{22} & r_{23} & r_{24} \\ 0 & 0 & a_{33}^{(2)} & a_{34}^{(2)} \\ 0 & 0 & a_{43}^{(2)} & a_{44}^{(2)} \\ 0 & 0 & a_{53}^{(2)} & a_{54}^{(2)} \\ 0 & 0 & a_{63}^{(2)} & a_{64}^{(2)} \end{bmatrix}$$

Householder QR Factorization

- Repeat the process on the third column

$$\mathbf{H}_3\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ 0 & r_{22} & r_{23} & r_{24} \\ 0 & 0 & r_{33} & r_{34} \\ 0 & 0 & 0 & a_{44}^{(2)} \\ 0 & 0 & 0 & a_{54}^{(2)} \\ 0 & 0 & 0 & a_{64}^{(2)} \end{bmatrix}$$

- One more should do it

$$\mathbf{H}_4\mathbf{H}_3\mathbf{H}_2\mathbf{H}_1\mathbf{A} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ 0 & r_{22} & r_{23} & r_{24} \\ 0 & 0 & r_{33} & r_{34} \\ 0 & 0 & 0 & r_{44} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Householder QR Factorization

- Algorithm for a Householder **QR** factorization

function $\mathbf{A}$ = houseqr($\mathbf{A}$)
% houseqr: Overwrite $\mathbf{A} \in \Re^{m \times n}$ with the product
% $\mathbf{QR}$ where $\mathbf{Q} \in \Re^{m \times m}$ is orthogonal and
% $\mathbf{R} \in \Re^{m \times n}$ is upper triangular. On return,
% the essential part of $\mathbf{Q}$ is stored in the lower triangular
% part of $\mathbf{A}$ and $\mathbf{R}$ is stored in the upper triangular part.

for $j = 1 : n$
  $\mathbf{v}$(j:m) = house($\mathbf{A}$(j:m,j));
  $\mathbf{A}$(j:m,j:n) = row.house($\mathbf{A}$(j:m,j:n), $\mathbf{v}$(j:m));
  if $j < m$
    $\mathbf{A}$(j+1:m,j) = $\mathbf{v}$(j+1:m);
  end
end

Householder QR Factorization

- As described in Example 2.4,

$$\mathbf{H}_j = \mathbf{I} - 2\frac{\mathbf{v}^{(j)}\left(\mathbf{v}^{(j)}\right)^T}{\left(\mathbf{v}^{(j)}\right)^T\mathbf{v}^{(j)}} \tag{2a}$$

  - $\mathbf{v}^{(j)}$ is the Householder vector $\mathbf{v}$ used at step j
  - $\mathbf{v}^{(j)}$ has the form

$$\mathbf{v}^{(j)} = [0, 0, ..., 0, 1, v_{j+1}^{(j)}, ..., v_m^{(j)}]^T \tag{2b}$$

- Normalize the Householder vector so that $v_j^{(j)} = 1$
  - This requires modification of the function *house* of Section 4.2. All components of $\mathbf{v}$ are divided by $v(1)$
  - The renormalization saves a storage location and allows $\mathbf{v}^{(j)}$ to be stored in the lower part of $\mathbf{A}$

- Upon completion of the algorithm

$$\mathbf{A} = \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} \\ v_2^{(1)} & r_{22} & r_{23} & r_{24} \\ v_3^{(1)} & v_3^{(2)} & r_{33} & r_{34} \\ v_4^{(1)} & v_4^{(2)} & v_4^{(3)} & r_{44} \\ v_5^{(1)} & v_5^{(2)} & v_5^{(3)} & v_5^{(4)} \\ v_6^{(1)} & v_6^{(2)} & v_6^{(3)} & v_6^{(4)} \end{bmatrix} \tag{2c}$$

Householder QR Factorization

- $\mathbf{Q}^T = \mathbf{H}_n \mathbf{H}_{n-1} \cdots \mathbf{H}_1$ so

$$\mathbf{Q} = \mathbf{H}_1 \mathbf{H}_2 \cdots \mathbf{H}_n \tag{3}$$

  - $\mathbf{Q}$ rarely needs explicit construction

- The factorization requires about $2n^2(m - n/3)$ FLOPs (multiplications plus additions)
  - With $m = n$ we require about $4n^3/3$ FLOPs
  - Gaussian elimination requires about $2n^3/3$ FLOPs

- With roundoff, we compute

$$\hat{\mathbf{Q}}^T(\mathbf{A} + \delta\mathbf{A}) = \hat{\mathbf{R}}$$

  - $\hat{\mathbf{Q}}$ is *exactly* orthogonal
  - $\hat{\mathbf{R}}$ is upper triangular
  - The perturbation $||\delta\mathbf{A}||_2 \approx u||\mathbf{A}||_2$
  - This is acceptable

Givens QR Factorization

- We can also use Givens rotations to construct the **QR** decomposition
  - The order of the reduction is
  - $\times$ stands for a nonzero entry
  - The numbers indicate the rows that are rotated

$$\mathbf{A} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} = \begin{matrix} \\ \\ \\ 3 \\ 4 \end{matrix} \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \end{bmatrix} = \begin{matrix} 2 \\ 3 \\ \\ \\ \end{matrix} \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}$$

$$\mathbf{A} = \begin{matrix} 1 \\ 2 \\ \\ \\ \end{matrix} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix} = \begin{matrix} \\ \\ 3 \\ 4 \end{matrix} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \end{bmatrix} = \begin{matrix} 2 \\ 3 \\ \\ \\ \end{matrix} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{bmatrix}$$

$$\mathbf{A} = \begin{matrix} \\ \\ 3 \\ 4 \end{matrix} \begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix}$$

Givens QR Factorization

- Algorithm for the Givens **QR** factorization

  function $\mathbf{A}$ = givensqr($\mathbf{A}$)
  % givensqr: Reduce $\mathbf{A} \in \Re^{m \times n}$ to upper triangular
  % form by the Givens **QR** procedure where $\mathbf{Q} \in \Re^{m \times m}$
  % is orthogonal and $\mathbf{R} \in \Re^{m \times n}$ is upper triangular.
  % On return, $\mathbf{R}$ is stored in the upper triangular part of $\mathbf{A}$.

  ```
  for j = 1:n
     for i = m: -1: j + 1
        [c,s] = givens(A(i-1,j), A(i,j));
        A(i-1:i,j:n) = row.rot(A(i-1:i,j:n), c, s);
     end
  end
  ```

  – The procedure does not save $\mathbf{Q}$

  – The factorization requires about $3n^2(m - n/3)$ multiplications and additions

    * Reflections require $2n^2(m - n/3)$ FLOPs
    * Reflections are generally preferred

  – Let $\mathbf{G}_i = \mathbf{G}(i, i-1, \theta)$, then

$$\mathbf{Q} = \underbrace{(\mathbf{G}_m \mathbf{G}_{m-1} \cdots \mathbf{G}_2)}_{1\ st\ col.} \underbrace{(\mathbf{G}_m \cdots \mathbf{G}_3)}_{2\ nd\ col.} \cdots \underbrace{(\mathbf{G}_m)}_{n\ th\ col.}$$

Givens QR Factorization

- *Example 1.* Obtain the **QR** factorization of

$$\mathbf{A} = \begin{bmatrix} 3 & 2 & 1 \\ 2 & -3 & 4 \\ 5 & 1 & -1 \\ 7 & 4 & 2 \end{bmatrix}$$

  - Rotating the third and fourth rows using givens(5,7)

$$c = -0.5812, \qquad s = 0.8137$$

  - Applying row.rot to $\mathbf{A}(3:4, 1:3)$ yields

$$\mathbf{A}^{(1)} = \begin{bmatrix} 3.0000 & 2.0000 & 1.0000 \\ 2.0000 & -3.0000 & 4.0000 \\ -8.6023 & -3.8362 & -1.0462 \\ 0 & -1.5112 & -1.9762 \end{bmatrix}$$

  - The Givens matrix corresponding to this rotation is

$$\mathbf{G}(3, 4, \theta)^T = \mathbf{G}_4^T$$

$$= \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c & -s \\ 0 & 0 & s & c \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -0.5812 & -0.8137 \\ 0 & 0 & 0.8137 & -0.5812 \end{bmatrix}$$

  - We may check that $\mathbf{G}_4^T \mathbf{A} = \mathbf{A}^{(1)}$

Givens QR Factorization

- Rotate the second and third rows using givens(2.0000, -8.6023)

$$c = 0.2265, \qquad s = 0.9740$$

  - Applying row.rot to $\mathbf{A}^{(1)}(2:3, 1:3)$ yields

$$\mathbf{A}^{(2)} = \begin{bmatrix} 3.0000 & 2.0000 & 1.0000 \\ 8.8318 & 3.0571 & 1.9249 \\ 0 & -3.7908 & 3.6592 \\ 0 & -1.5112 & -1.9762 \end{bmatrix}$$

  - The rotation matrix is

$$\mathbf{G}_3^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.2265 & -0.9740 & 0 \\ 0 & 0.9740 & 0.2265 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

  - We may check that $\mathbf{G}_3^T \mathbf{G}_4^T \mathbf{A} = \mathbf{A}^{(2)}$

Givens QR Factorization

- Rotate the first and second rows using givens(3.0000, 8.8318)

$$c = -0.3216, \qquad s = 0.9469$$

  - Applying row.rot to $\mathbf{A}^{(2)}(1:2, 1:3)$ yields

$$\mathbf{A}^{(3)} = \begin{bmatrix} -9.3274 & -3.5380 & -2.1442 \\ 0 & 0.9104 & 0.3278 \\ 0 & -3.7908 & 3.6592 \\ 0 & -1.5112 & -1.9762 \end{bmatrix}$$

  - The Givens matrix

$$\mathbf{G}_2^T = \begin{bmatrix} -0.3216 & -0.9469 & 0 & 0 \\ 0.9469 & -0.3216 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

  - The first column has been reduced

Givens QR Factorization

- Rotate the third and fourth rows using givens(-3.7908, -1.5112)

$$c = 0.9289, \qquad s = -0.3703$$

  - Applying row.rot to $\mathbf{A}^{(3)}(3:4, 2:3)$ yields

$$\mathbf{A}^{(4)} = \begin{bmatrix} -9.3274 & -3.5380 & -2.1442 \\ 0 & 0.9104 & 0.3278 \\ 0 & -4.0809 & 2.6672 \\ 0 & 0 & -3.1908 \end{bmatrix}$$

  - The Givens matrix

$$\mathbf{G}_4^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0.9289 & -0.3703 \\ 0 & 0 & 0.3703 & 0.9289 \end{bmatrix}$$

- Rotate the second and third rows using givens(0.9104, -4.0809)

$$c = 0.2177, \qquad s = 0.9760$$

  - Applying row.rot to $\mathbf{A}^{(4)}(2:3, 2:3)$ yields

$$\mathbf{A}^{(5)} = \begin{bmatrix} -9.3274 & -3.5380 & -2.1442 \\ 0 & 4.1812 & -2.5318 \\ 0 & 0 & 0.9007 \\ 0 & 0 & -3.1908 \end{bmatrix}$$

  - The Givens matrix

$$\mathbf{G}_3^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0.2177 & -0.9760 & 0 \\ 0 & 0.9760 & 0.2177 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

  - The second column is done

The Last Rotation

- Rotate the third and fourth rows using givens(0.9007, -3.1908)

$$c = 0.2717, \qquad s = 0.9624$$

  - Applying row.rot to $\mathbf{A}^{(5)}(3:4, 3)$ yields

$$\mathbf{A}^{(6)} = \begin{bmatrix} -9.3274 & -3.5380 & -2.1442 \\ 0 & 4.1812 & -2.5318 \\ 0 & 0 & 3.3154 \\ 0 & 0 & 0 \end{bmatrix}$$

  - The Givens matrix

$$\mathbf{G}_4^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0.2717 & -0.9624 \\ 0 & 0 & 0.9624 & 0.2717 \end{bmatrix}$$

The Factored Form

- The factored matrix

$$\mathbf{R} = \begin{bmatrix} -9.3274 & -3.5380 & -2.1442 \\ 0 & 4.1812 & -2.5318 \\ 0 & 0 & 3.3154 \\ 0 & 0 & 0 \end{bmatrix}$$

- The orthogonal matrix
  - We have

$$\mathbf{Q}^T = \underbrace{(\mathbf{G}_4)}_{3\ rd\ col.}\ \underbrace{(\mathbf{G}_3^T\mathbf{G}_4^T)}_{2\ nd\ col.}\underbrace{(\mathbf{G}_2^T\mathbf{G}_3^T\mathbf{G}_4^T)}_{1\ st\ col.}$$

$$\mathbf{Q} = \begin{bmatrix} -0.3216 & 0.2062 & 0.2511 & 0.8894 \\ -0.2144 & -0.8989 & 0.3813 & 0.0232 \\ -0.5361 & -0.2144 & -0.8121 & 0.0851 \\ -0.7505 & 0.3216 & 0.3635 & -0.4486 \end{bmatrix}$$

  - Check that $\mathbf{QR} = \mathbf{A}$
  - Check that $\mathbf{Q}^T\mathbf{Q} = \mathbf{I}$

Properties of the QR Factorization

- **Theorem 1:** Let $\mathbf{A} \in \Re^{m\times n}$ have rank n with $m \geq n$. Let $\mathbf{A} = \mathbf{QR}$, then

$$\text{span}\{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_k\} = \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_k\}, \qquad k = 1:n \tag{4a}$$

  - $\mathbf{A} = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n]$ etc.
  - Let $\mathbf{Q}_n = [\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_n]$, $\mathbf{Q}_{m-n} = [\mathbf{q}_{n+1}, \mathbf{q}_{n+2}, \cdots, \mathbf{q}_m]$
  - Then

$$\text{range}(\mathbf{A}) = \text{range}(\mathbf{Q}_n) \tag{4b}$$

$$\text{range}(\mathbf{A})^{\perp} = \text{range}(\mathbf{Q}_{m-n}) \tag{4c}$$

    * The $\perp$ denotes the orthogonal complement
  - In addition

$$\mathbf{A} = \mathbf{Q}_n\mathbf{R}_n, \qquad \mathbf{R}_n = \mathbf{R}(1:n, 1:n) \tag{4d}$$

- *Remark:*

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_n \\ \mathbf{0} \end{bmatrix} \qquad \mathbf{Q} = \begin{bmatrix} \mathbf{Q}_n & \mathbf{Q}_{m-n} \end{bmatrix}$$

  - Thus,

$$\mathbf{A} = \mathbf{QR} = \begin{bmatrix} \mathbf{Q}_n & \mathbf{Q}_{m-n} \end{bmatrix} \begin{bmatrix} \mathbf{R}_n \\ \mathbf{0} \end{bmatrix} = \mathbf{Q}_n\mathbf{R}_n$$

- *Proof:* From (1)

$$\mathbf{a}_k = \sum_{j=1}^{k} r_{jk}\mathbf{q}_j \in \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_k\} \tag{5}$$

- Thus,

$$\text{span}\{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_k\} \subseteq \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_k\}$$

Fat and Skinny QRs

- But rank($\mathbf{A}$) = n; thus,

$$\dim(\text{span}\{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_k\}) = k$$

  So

$$\text{span}\{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_k\} = \text{span}\{\mathbf{q}_1, \mathbf{q}_2, \cdots, \mathbf{q}_k\}$$

- Thus, (4a) is satisfied
- The rest of the Theorem follows directly □
- We call (4c) the *thin* or *reduced* **QR** *factorization* of $\mathbf{A}$
- **Theorem 2:** Let $\mathbf{A} \in \Re^{m \times n}$ have rank n, then the thin **QR** factorization (4c) is unique.
  - $\mathbf{R}_n$ is upper triangular with positive diagonal entries
  - Consider the Cholesky factorization of

$$\mathbf{A}^T\mathbf{A} = \mathbf{L}\mathbf{L}^T \tag{6a}$$

    * $\mathbf{L}$ is lower triangular
  - Then

$$\mathbf{R}_n = \mathbf{L}^T \tag{6b}$$

- *Proof:* Consider

$$\mathbf{A}^T\mathbf{A} = \mathbf{R}_n^T\mathbf{Q}_n^T\mathbf{Q}_n\mathbf{R}_n = \mathbf{R}_n^T\mathbf{R}_n$$

  - Comparing this with (6a) yields (6b)
  - The Cholesky factorization is unique
  - From (4d) $\mathbf{Q}_n = \mathbf{A}\mathbf{R}_n^{-1}$; hence, $\mathbf{Q}_n$ is unique □

The Condition Number of a Rectangular Matrix

- What is the condition number of an $m \times n$ matrix?
- **Theorem 3:** Let $\mathbf{A} \in \Re^{n \times n}$, then
  - The eigenvalues λ_i, $i = 1 : n$, of $\mathbf{A}^T\mathbf{A}$ and the singular values σ_i, $i = 1 : n$, satisfy

$$\lambda_i = \sigma_i^2, \qquad i = 1 : n \tag{7a}$$

  - The eigenvectors $\mathbf{x}_i$ of $\mathbf{A}^T\mathbf{A}$ and the singular vectors $\mathbf{v}_i$ of $\mathbf{A}$ satisfy

$$\mathbf{x}_i = \mathbf{v}_i, \qquad i = 1 : n \tag{7b}$$

  - The Euclidean norm

$$||\mathbf{A}||_2 = \sqrt{\rho(\mathbf{A}^T\mathbf{A})} = \sigma_1 \tag{7c}$$

    * The spectral radius $\rho(\mathbf{A}^T\mathbf{A})$ is the largest eigenvalue λ_1 of $\mathbf{A}^T\mathbf{A}$
    * σ_1 is the largest singular value of $\mathbf{A}$
  - The condition number of $\mathbf{A}$ in the Euclidean norm satisfies

$$\kappa_2(\mathbf{A}) = \frac{\sigma_1(\mathbf{A})}{\sigma_n(\mathbf{A})} \tag{7d}$$

The Condition Number of a Rectangular Matrix

- *Proof:*

- We can use this as a definition of the condition number for a rectangular matrix
  - An $O(\epsilon)$ perturbation in $\mathbf{A}$ introduces $O(\epsilon\kappa_2(\mathbf{A}))$ perturbations in $\mathbf{Q}_n$ and $\mathbf{R}_n$
    - cf. Stewart (1993), On the perturbation of LU Cholesky and QR factorizations, *SIAM J. Matrix. Anal.*, **14**, 1141-1145