Math 2270-1

Notes of 09/18/19

Matrix Factorizations

- A **factorization** of a matrix A is obtained by expressing A as a product of several (usually 2 or 3) factors.
- There are very many widely used matrix factorizations and in this class we will encounter just a few of them.
- To begin with, suppose A is a (square) invertible matrix and you want to solve the linear system
$$A\mathbf{x} = \mathbf{b}$$
for several right hand sides
$$\mathbf{b} = \ \mathbf{b}_1, \mathbf{b}_2, \ldots, \mathbf{b}_p\,,$$
giving solutions
$$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\,,$$
where
$$A\mathbf{x}_i = \mathbf{b}_i, \qquad i = 1, \ldots, p.$$

For the moment, and for simplicity, let us assume that the pivots are all non-zero, i.e.,

we do not need to apply row interchanges. We'll discuss pivoting later.

- We know several ways of solving those linear systems.

1. Solve each system independently and from scratch. That is obviously wasteful!

2. Augment the matrix A with all right hand sides, to get the augmented matrix

$$[A \quad \mathbf{b}_1 \quad \mathbf{b}_2 \quad \dots \quad \mathbf{b}_p]$$

and reduce to the reduced row echelon form

$$[I \quad \mathbf{x}_1 \quad \mathbf{x}_2 \quad \dots \quad \mathbf{x}_p]$$

But note that we need to know all right hand sides before solving any of the linear systems. In applications we often get a new right hand side only after solving the most recent of those systems.

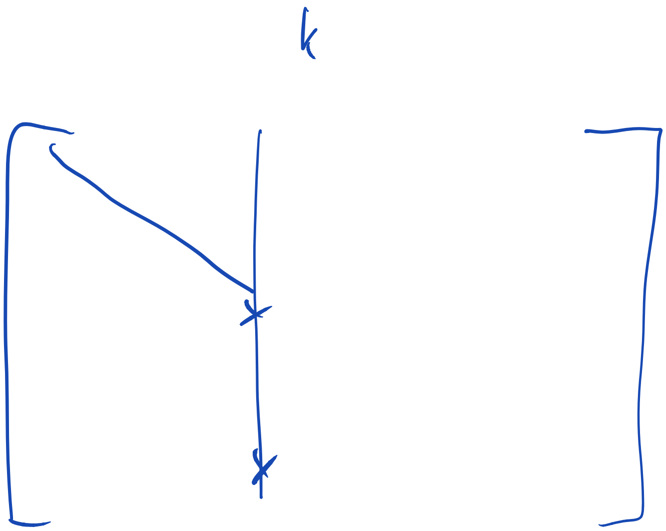
3. Compute A^{-1} and then get

$$\mathbf{x}_i = A^{-1}\mathbf{b}_i$$

when we need it.

4. Apply row operations to reduce A to (unreduced) row echelon form and keep track of the multipliers. Then, using the stored multipliers, process each right hand side, and use back substitution.

where do we store the multipliers?



- Our focus today is on an alternative approach. Factor A as

$$A = LU \tag{1}$$

where

L is **unit lower triangular**, i.e.,

$$l_{ii} = 1, \quad i = 1, 2, \dots n \quad \text{and} \quad j < i \quad \Longrightarrow \quad \overset{l}{\cancel{a}}_{ij} = 0$$

U is **upper triangular**, i.e.,

$$\cancel{l_{ii} = 1,} \quad i = 1, 2, \dots n \quad \text{and} \quad j > i \quad \Longrightarrow \quad \overset{u}{\cancel{a}}_{ij} = 0$$

- In other words, denoting possibly non-zero entries by x, L and U are of the form:

$$L = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ x & 1 & 0 & \dots & 0 & 0 \\ x & x & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ x & x & x & \dots & 1 & 0 \\ x & x & x & \dots & x & 1 \end{bmatrix}$$

and

$$U = \begin{bmatrix} x & x & x & \dots & x & x \\ 0 & x & x & \dots & x & x \\ 0 & 0 & x & \dots & x & x \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & x & x \\ 0 & 0 & 0 & \dots & 0 & x \end{bmatrix}$$

- Given the matrix factorization (1) we solve the system $Ax = LUx = b$ in two steps:

1. solve: $Lz = b$ Forward Substitution
2. solve: $Ux = z$ Backward Substitution

- Example: Let

$$A = \begin{bmatrix} 1 & -1 & 1 \\ 2 & 0 & 1 \\ 4 & 2 & 4 \end{bmatrix}, L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 4 & 3 & 1 \end{bmatrix}, \quad \text{and} \quad U = \begin{bmatrix} 1 & -1 & 1 \\ 0 & 2 & -1 \\ 0 & 0 & 3 \end{bmatrix}$$

- Then $A = LU$:

$$\begin{array}{ccc} & \begin{bmatrix} 1 & -1 & 1 \\ 0 & 2 & -1 \\ 0 & 0 & 3 \end{bmatrix} & = U \\ L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 4 & 3 & 1 \end{bmatrix} & \begin{bmatrix} 1 & -1 & 1 \\ 2 & 0 & 1 \\ 4 & 2 & 4 \end{bmatrix} & = A \end{array}$$

- moreover, let

$$\mathbf{x} = \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}$$

- Then

$$A\mathbf{x} = \begin{bmatrix} 4 \\ 3 \\ 4 \end{bmatrix}$$

- Find $\mathbf{x}$ by using the LU factorization.

$$b = \begin{bmatrix} 4 \\ 3 \\ 4 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 4 & 3 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 4 \\ 3 \\ 4 \end{bmatrix}$$

$z_1 = 4$

$2z_1 + z_2 = 3 \qquad z_2 = -5$

$4z_1 + 3z_2 + z_3 = 4$

$z_3 = 4 - 16 + 15 = 3$

$$z = \begin{bmatrix} 4 \\ -5 \\ 3 \end{bmatrix}$$

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

$x_3 = 1$

$2x_2 - 1 = -5 \qquad x_2 = -2$

$x_1 + 2 + 1 = 4 \qquad x_1 = 1$

- OK, and how would we have done it the old way?

$$\begin{bmatrix} 1 & -1 & 1 \\ 2 & 0 & 1 \\ 4 & 2 & 4 \end{bmatrix} \longrightarrow \begin{bmatrix} 1 & -1 & 1 \\ 2 & 2 & -1 \\ 4 & 6 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 1 & -1 & 1 \\ 2 & 2 & -1 \\ 4 & 3 & 3 \end{bmatrix}$$

$$\begin{bmatrix} 4 \\ 3 \\ 4 \end{bmatrix} \rightarrow \begin{bmatrix} 4 \\ -5 \\ -12 \end{bmatrix} \rightarrow \begin{bmatrix} 4 \\ -5 \\ 3 \end{bmatrix}$$

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

Actually, **Reduction to r.e.f. computes the LU factorization!**

- the two procedures are equivalent!
- The standard argument to show this is a mess that involves "elementary matrices" and their inverses, and generous use of groups of three dots ...
- See textbook for an argument along those lines.
- However, Gil Strang of MIT came up with a beautifully simple argument.
- Consider the evolution of the working array during Gaussian Elimination, for a 4×4 system.
- The letter x denotes an entry in the working array. The symbol $\otimes$ denotes an entry that is final and no longer changed in the process. The letter m denotes the multipliers, stored in the lower part of the working array.

- We get

$$\begin{bmatrix} \otimes & \otimes & \otimes & \otimes \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix} \longrightarrow \begin{bmatrix} \otimes & \otimes & \otimes & \otimes \\ m_{21} & \otimes & \otimes & \otimes \\ m_{31} & x & x & x \\ m_{41} & x & x & x \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} \otimes & \otimes & \otimes & \otimes \\ m_{21} & \otimes & \otimes & \otimes \\ m_{31} & m_{32} & \otimes & \otimes \\ m_{41} & m_{42} & x & x \end{bmatrix}$$

$$\longrightarrow \begin{bmatrix} \otimes & \otimes & \otimes & \otimes \\ m_{21} & \otimes & \otimes & \otimes \\ m_{31} & m_{32} & \otimes & \otimes \\ m_{41} & m_{42} & m_{43} & \otimes \end{bmatrix}$$

- Let's denote row i of a matrix A by $r_i(A)$ and consider in particular the third row of the working array. We get

$$r_3(U) = r_3(A) - m_{31}r_1(U) - m_{32}r_2(U)$$

- This can be rewritten as

$$r_3(A) = m_{31}r_1(U) + m_{32}r_2(U) + r_3(U)$$

That last equation is exactly what we get in the matrix multiplication $A = LU$!

$$
\begin{array}{cc}
 & \begin{bmatrix} r_1(U) \\ r_2(U) \\ r_3(U) \\ r_4(U) \end{bmatrix} = U \\
\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ m_{21} & 1 & 0 & 0 \\ m_{31} & m_{32} & 1 & 0 \\ m_{41} & m_{42} & m_{43} & 1 \end{bmatrix}}_{= L} & \begin{bmatrix} r_1(A) \\ r_2(A) \\ r_3(A) \\ r_4(A) \end{bmatrix} = A
\end{array}
$$

- Clearly, this applies in general, not just to the third row of a 4×4 matrix!
- $A = LU$, L is unit lower triangular, U is upper triangular.

Pivoting

- We understand pivoting from a computational point of view, but we also want to describe it in terms of matrices.
- A **permutation matrix** is a square matrix that is all zero except that it has one entry equal to 1 in each row and each column.
- Another view is that a permutation matrix is obtained by permuting the rows or the columns of the identity matrix.
- Multiplying a matrix A with a permutation matrix from the left permutes the rows of A and multiplying from the right permutes the columns of A.
- Example: Let

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \quad \text{and} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Then:

$$\begin{array}{cccc} & & \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & = P \\ & A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} & \begin{bmatrix} 2 & 1 \\ 4 & 3 \end{bmatrix} & = AP \\ P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \begin{bmatrix} 3 & 4 \\ 1 & 2 \end{bmatrix} & = PA & \end{array}$$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$x = 2 \quad y = 1$

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

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

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

$P^{-1} = P^T$

$P^T P = I$

On Computing the Inverse

It usually is a bad idea to compute an inverse matrix, for these reasons:

0. You don't need an explicit expression for the inverse to multiply with it, since $A^{-1}\mathbf{b}$ is the solution of $A\mathbf{x} = \mathbf{b}$. So instead of multiplying with A^{-1} you can just solve a linear system!

1. Computing A^{-1} requires more (actually three times as much for large values of n) computational work than computing the LU factorization.

2. A major problem in numerical procedures is the propagation of round-off errors, since numbers can be expressed only approximately on a computer. The inverse of a matrix is affected more than the LU factorization by such errors.

3. Most importantly, but also most subtly, matrix inversion destroys sparsity, whereas the LU factorization has a better chance to preserve it. A matrix is sparse if most of its entries are zero.

Factorization and Block Matrices

- Let's combine the last two topics, partitioned matrices, and matrix factorizations.
- Suppose

$$A = \begin{array}{c c} & \begin{array}{cc} n-1 & 1 \end{array} \\ \begin{array}{c} n-1 \\ 1 \end{array} & \begin{pmatrix} \hat{A} & \mathbf{c} \\ \mathbf{r}^T & a_{nn} \end{pmatrix} \end{array}$$

  and suppose we have computed the LU factorization
  $$\hat{A} = \hat{L}\hat{U}$$
  of $\hat{A}$. Without starting from scratch, can you compute the LU factorization of A?
- Try

$$L = \begin{bmatrix} \hat{L} & 0 \\ \hat{\mathbf{y}}^T & 1 \end{bmatrix} \quad \text{and} \quad U = \begin{bmatrix} \hat{U} & 0 \\ \mathbf{x} & \xi \end{bmatrix}.$$

  How do you pick $\mathbf{x} \in \mathbb{R}^{n-1}$, $\mathbf{y} \in \mathbb{R}^{n-1}$, and $\xi \in \mathbb{R}$? What can go wrong?

- **Example and Exercise:** The $n \times n$ matrix

$$A = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \tag{2}$$

occurs frequently in the solution of second order ordinary differential equations.

a. Show that

$$A^{-1} = [\, x_{ij} \,] \tag{3}$$

where

$$x_{ij} = \begin{cases} \dfrac{(n+1-j)i}{n+1} & i = 1, 2, \ldots, j \\ \dfrac{(n+1-i)j}{n+1} & i = j+1, \ldots, n. \end{cases} \tag{4}$$

b. Show that

$$A = LU$$

where $L = [\, l_{ij} \,]$ is unit lower triangular and $U = [\, u_{ij} \,]$ is upper triangular and

$$l_{ii} = 1, \quad l_{i,i-1} = -\frac{i-1}{i}, \quad u_{ii} = \frac{i+1}{i}, \quad \text{and} \quad u_{i,i+1} = -1. \tag{5}$$

c. Discuss the differences between solving $Ax = b$ by multiplying with the inverse, and by applying backward and forward substitution to the LU factorization.

• Example. In the case $n = 10$ we get

$$A^{-1} = \frac{1}{11}\begin{bmatrix} 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 9 & 18 & 16 & 14 & 12 & 10 & 8 & 6 & 4 & 2 \\ 8 & 16 & 24 & 21 & 18 & 15 & 12 & 9 & 6 & 3 \\ 7 & 14 & 21 & 28 & 24 & 20 & 16 & 12 & 8 & 4 \\ 6 & 12 & 18 & 24 & 30 & 25 & 20 & 15 & 10 & 5 \\ 5 & 10 & 15 & 20 & 25 & 30 & 24 & 18 & 12 & 6 \\ 4 & 8 & 12 & 16 & 20 & 24 & 28 & 21 & 14 & 7 \\ 3 & 6 & 9 & 12 & 15 & 18 & 21 & 24 & 16 & 8 \\ 2 & 4 & 6 & 8 & 10 & 12 & 14 & 16 & 18 & 9 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{bmatrix}$$

- On the other hand, omitting the zero entries,

$$L = \frac{1}{11}\begin{bmatrix} 1 \\ -1/2 & 1 \\ & -2/3 & 1 \\ & & -3/4 & 1 \\ & & & -4/5 & 1 \\ & & & & -5/6 & 1 \\ & & & & & -6/7 & 1 \\ & & & & & & -7/8 & 1 \\ & & & & & & & -8/9 & 1 \\ & & & & & & & & -9/10 & 1 \end{bmatrix}$$

and

$$U = \begin{bmatrix} 2 & -1 \\ & 3/2 & -1 \\ & & 4/3 & -1 \\ & & & 5/4 & -1 \\ & & & & 6/5 & -1 \\ & & & & & 7/6 & -1 \\ & & & & & & 8/7 & -1 \\ & & & & & & & 9/8 & -1 \\ & & & & & & & & 10/9 & -1 \\ & & & & & & & & & 11/10 \end{bmatrix}$$