

Today:

Announcements:

- HW2 due, HW3 out
- Examlet / next week
- MOSS / collab. policy
- IETF

Fixing nonexistence of LU

What does LU with permutations process look like?

$$M_3 P_3 M_2 P_2 M_1 P_1 A = U$$

$$A = \underbrace{(M_3 P_3 M_2 P_2 M_1 P_1)^{-1}}_L U$$

Demo: LU with Partial Pivoting (Part I)

What about the L in LU?

Sort out what LU with pivoting looks like. Have: $M_3 P_3 M_2 P_2 M_1 P_1 A = U$.

$$L_3 := M_3 \quad | \quad L_2 := P_3 M_2 P_3^{-1} \quad | \quad L_1 := P_3 P_2 M_1 P_2^{-1} P_3^{-1}$$

$$\underline{L_3 L_2 L_1} \quad \underline{P_3 P_2 P_1}$$

$$\cancel{M_3} \quad \cancel{P_3} \quad \cancel{M_2} \quad \cancel{P_3^{-1}} \quad \cancel{P_3 P_2} \quad \cancel{M_1} \quad \cancel{P_2^{-1}} \quad \cancel{P_3^{-1}} \quad P_1 A = U$$

$$\underbrace{P_3 P_2 P_1}_P A = \underbrace{(L_1^{-1} L_2^{-1} L_3^{-1})}_L U$$

$$\underline{M_3 P_3} \quad \underline{M_2 P_2} \quad \underline{M_1 P_1} A = U$$

Demo: LU with Partial Pivoting (Part II)

$$\rightarrow PA = LU$$

Computational Cost

$$[AB]_{ij} = \sum_k A_{ik} B_{kj}$$

What is the computational cost of multiplying two $n \times n$ matrices?

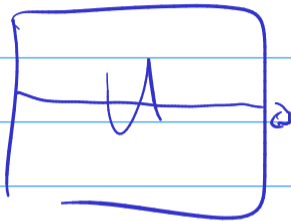
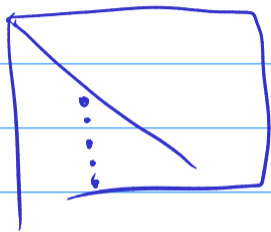
$$O(n^3)$$

$$\begin{array}{l} n, A \rightarrow O(n^2) \\ PA \\ \hline O(n) \end{array}$$

What is the computational cost of carrying out LU factorization on an $n \times n$ matrix?

$$\underbrace{O(n)}_{\text{\# columns}} \cdot \underbrace{O(n^2)}_{\text{cost of applying on din}} = O(n^3)$$

Demo: Complexity of Mat-Mat multiplication and LU



More cost concerns

What's the cost of solving $Ax = b$?

$$\left. \begin{array}{l} O(n^3) \text{ for } LU \\ 2 \cdot O(n^2) \text{ for } fu/bw \rightarrow O(n^2) \end{array} \right\} O(n^3)$$

What's the cost of solving $Ax = b_1, b_2, \dots, b_n$?

$$\left. \begin{array}{l} O(n^3) \text{ for } LU \\ \rightarrow n \cdot O(n^2) \text{ for } fu/bw \end{array} \right\} O(n^3)$$

What's the cost of finding A^{-1} ?

$$Ax = I$$

\uparrow
 A^{-1}

$$\begin{aligned} PA &= LU \\ A &= P^T LU \\ LUx &= Pb \end{aligned}$$

Solving w. m RHS:

$$O(h^3) + O(m \cdot h^2)$$

Cost: Worrying about the Constant, BLAS

$O(n^3)$ really means

$$\alpha \cdot n^3 + \beta \cdot n^2 + \gamma \cdot n + \delta.$$

All the non-leading and constants terms swept under the rug. But: at least the leading constant ultimately matters.

Getting that constant to be small is surprisingly hard, even for something deceptively simple such as matrix-matrix multiplication.

Idea: Rely on library implementation: *BLAS* (Fortran)

Level 1 $z = \alpha x + y$ vector-vector operations

$O(n)$

?axpy

Level 2 $z = Ax + y$ matrix-vector operations

$O(n^2)$

?gemv

Level 3 $C = AB + \beta C$ matrix-matrix operations

$O(n^3)$

?gemm, ?trsm



LAPACK

LAPACK: Implements 'higher-end' things (such as LU) using BLAS
Special matrix formats can also help save const significantly, e.g.

- ▶ banded
- ▶ sparse
- ▶ symmetric
- ▶ triangular

Sample routine names:

- ▶ dgesvd, zgesdd
- ▶ dgetrf, dgetrs

LU on Blocks: The Schur Complement

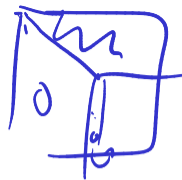
Given a matrix

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}, \quad \text{and } -CA^{-1}$$

can we do 'block LU' to get a *block triangular matrix*?

$$\begin{pmatrix} A & B \\ 0 & D - CA^{-1}B \end{pmatrix}$$

LU: Special cases



What happens if we feed a non-invertible matrix to LU?

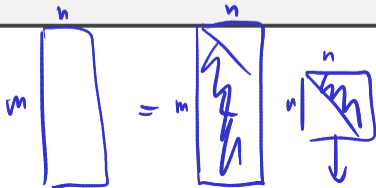
$$PA = LU \leftarrow \text{not inv.}$$

inv.
not invertible

What happens if we feed LU an $m \times n$ non-square matrices?

$$A = LU$$

$m \times n$ $m \times m$ $n \times n$



$m > n$; $m \times n$ $n \times n$
 $m < n$; $m \times m$ $m \times n$

Round-off Error in LU

Consider factorization of $\begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix}$ where $\epsilon < \epsilon_{\text{mach}}$:

Suppose $\epsilon_{\text{mach}} = 10^{-5}$
 $\epsilon = 10^{-5}$

▶ Without pivoting: $L = \begin{bmatrix} 1 & 0 \\ 1/\epsilon & 1 \end{bmatrix}$, $U = \begin{bmatrix} \epsilon & 1 \\ 0 & 1 - 1/\epsilon \end{bmatrix}$

▶ Rounding: $\text{fl}(U) = \begin{bmatrix} \epsilon & 1 \\ 0 & -1/\epsilon \end{bmatrix}$

▶ This leads to $L \text{fl}(U) = \begin{bmatrix} \epsilon & 1 \\ 1 & 0 \end{bmatrix}$, a backward error of $\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

Permuting the rows of A in partial pivoting gives $PA = \begin{bmatrix} 1 & 1 \\ \epsilon & 1 \end{bmatrix}$

▶ We now compute $L = \begin{bmatrix} 1 & 0 \\ \epsilon & 1 \end{bmatrix}$, $U = \begin{bmatrix} 1 & 1 \\ 0 & 1 - \epsilon \end{bmatrix}$, so $\text{fl}(U) = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$

▶ This leads to $L \text{fl}(U) = \begin{bmatrix} 1 & 1 \\ \epsilon & 1 + \epsilon \end{bmatrix}$, a backward error of $\begin{bmatrix} 0 & 0 \\ 0 & \epsilon \end{bmatrix}$.

Changing matrices

$$\begin{array}{l|l} Ax=b & Ax=b \\ Ax=c & \begin{array}{l} Cx=d \\ \uparrow \\ A+uv^T \end{array} \end{array}$$

Seen: LU cheap to re-solve if RHS changes. (Able to keep the expensive bit, the LU factorization) What if the *matrix* changes?

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^T A^{-1}}{1 + v^T A^{-1}u}$$

Demo: Sherman-Morrison

$$A^{-1} \vec{x}$$

solve $A \vec{z} = \vec{x}$

rank $uv^T = 1$

In-Class Activity: LU

In-class activity: LU and Cost

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Introduction

Sensitivity and Conditioning

Solving Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

What about non-square systems?

Specifically, what about linear systems with 'tall and skinny' matrices? (A: $m \times n$ with $m > n$) (aka *overdetermined* linear systems)

Specifically, any hope that we will solve those exactly?

