CS590C: Introduction to Computational Science

Lecture 3: Elementary Linear Algebra.

This lecture is intended to:

- ❏ Review basics of linear algebra
- ❏ Commonly used decompositions and linear system solution techniques (direct methods, Jacobi, Gauss-Siedel, and SOR), eigenvalues and eigenvectors.
- ❏ Some physical applications

Elementary matrix concepts:

- ❑ A matrix A is an $n \times m$ array of numbers (complex or real)
- ❑ Matrix addition: for matrices $A, B,$ and C,

  $C = A + B$, iff $c_{ij} = a_{ij} + b_{ij}$ $(i = 1 \text{ to } n, j = 1 \text{ to } m)$

- ❑ Multiplication of a matrix with a scalar:

  $D = sA$ iff $d_{ij} = s * a_{ij}$

- ❑ Matrix multiplication:

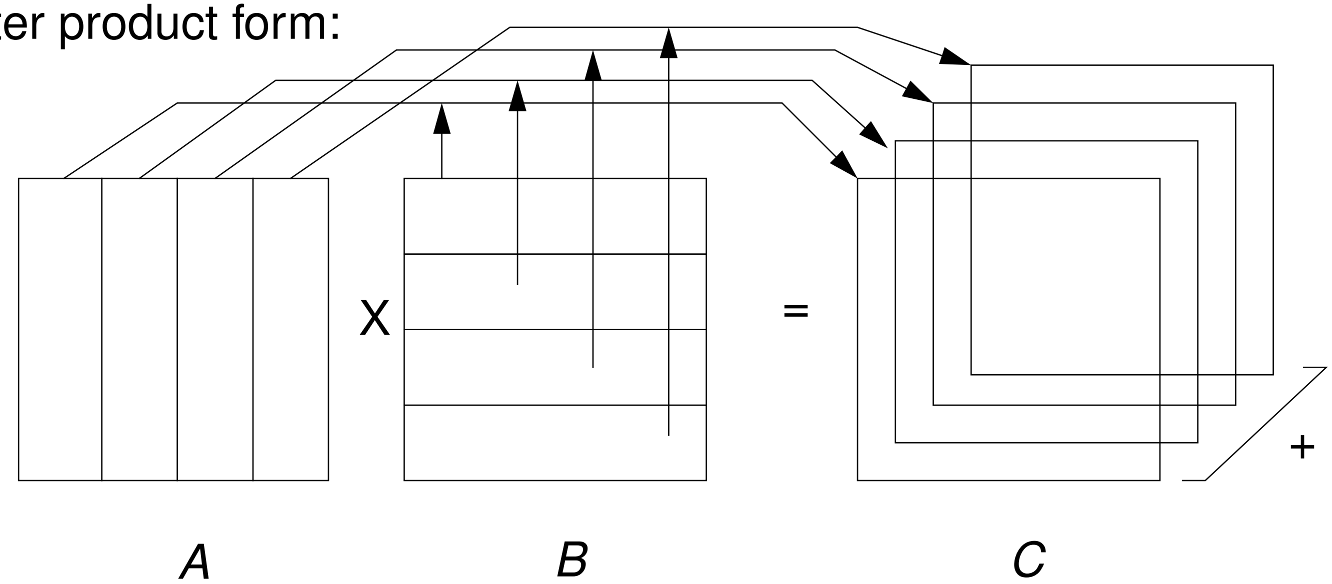
  Given matrices A_{nm} and B_{mp}

  $C = A.B$ iff c_{ij} = dot product($a_{i,*}, b_{*,j}$)

  (dot-product formulation)

Matrix multiplication:

- Outer product form:



- Blocked matrix multiply:

  Divide *A, B* into blocks and express each block of *C* as products of blocks of *A* and *B*.

Minimization of energy:

Why are linear systems so ubiquitous?

- They correspond to minimum energy states of many physical systems.

- For instance, given an expression for system energy of the form

$E = 0.5\ x^T A x - bx,$

- The minimum energy state is achieved by equating the first derivative to 0, i.e. $Ax - b = 0$.

- Remember, it is the minima only if the second derivative is positive (*hint: think positive definite systems*).

- Linear systems also arise in the solution of over-constrained systems using least squares ($A^T A x = A^T b$).

Linear systems of equations:

$$2x_1 + 4x_2 = 2$$
$$4x_1 + 11x_2 = 1$$

or $Ax = b$, where

$$A = \begin{bmatrix} 2 & 4 \\ 4 & 11 \end{bmatrix}, b = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

Solving the system:

Gaussian Elimination

$$2x_1 + 4x_2 = 2$$
$$3x_2 = -3$$

or $X_1 = 3$ *and* $X_2 = -1$.

Gaussian Elimination: A closer look.

- Transforms $Ax = b$ to $Ux = c$
(the solution x is identical for both systems since we have preserved right hand sides)

$$U = \begin{bmatrix} 2 & 4 \\ 0 & 3 \end{bmatrix}, c = \begin{bmatrix} 2 \\ -3 \end{bmatrix}$$

U is an upper triangular matrix, x can be determined using back-substitution.

- *Can we get back vector b from c?*

Collect the multipliers for the pivots and multiply it with b.

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

or $b = Lc$, where L is a lower-triangular matrix.

Gaussian Elimination: A closer look

Why did we do all this?

- Say we are given a matrix A and we need to solve it for multiple right hand sides b. (It happens very frequently in real problems).

- In this case, it is possible to determine L and U for matrix A without knowing vector b. Now to determine the value of x,

- First solve $Lc = b$, and then $Ux = c$.

- Advantage (each of the solves now requires only n^2 operations as opposed to n^3 operations required by elimination each time).

Gaussian Elimination: A closer look.

- In trying to solve Ax = b, we broke the problem down into

  $Ux = c$ and $Lc = b$
  or
  $LUx = b$.

But we had $Ax = b$,

- Therefore the result of Gaussian Elimination is factorization of matrix A into lower and upper triangular matrices. This factorization is sometimes also referred to as LU factorization.

- It is in fact possible to go further and diagonalize A completely, in which case, we will have A^{-1}. But we rarely need A^{-1}, instead, we need solutions to $Ax=b$. If we go further to determine A^{-1}, it is referred to as Gauss-Jordan Elimination.

Direct Factorization: A real application:

Consider the steady state temperature distribution in a one-dimensional metal rod.

The governing equation is

$$\frac{d^2T}{dx^2} = k$$

The metal rod is bounded at $x = 0$ and $x = 3$. The boundary conditions are $T = 100$ at $x = 0$, and $T = 0$ at $x = 3$.

Let us partition the rod into segments at $x = 0, 1, 2, 3$. Let us pick $k = 1$. We also know from elementary calculus that for this discretization,

$$\frac{d^2T}{dx^2} = 2T - T_1 - T_{-1}$$

Direct Factorization: A real application:

Inserting into the equation, we have

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} T0 \\ T1 \\ T2 \\ T3 \end{bmatrix} = \begin{bmatrix} 100 \\ 1 \\ 1 \\ 0 \end{bmatrix}$$

$$U = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 1.5 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix}, L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -0.5 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Solve this using forward and back substitution to determine T = (100, 67.67, 34.33, 0.0).

Factorization, observations:

- It is possible to divide the diagonal by the pivots in U.

- If A is symmetric, A can be factorized into LDU and $U = L^T$ Therefore $A = LDL^T$.

- If all pivots are positive, the matrix is referred to as positive definite.

- In this case, the diagonal matrix can be split by taking the square roots and included into the L matrix. In this case, the decomposition is $A = LL^T$.

- In many cases A is sparse (as noticed in the example). In such cases it is possible to save considerable time by being smart.

Linear Systems: Iterative Solvers:

We are trying to solve $Ax = b$,

Let us write $Ax = b$ as

$$Mx = Mx - Ax + b$$

or $Mx = (M-A)\ x + b$.

This equation forms the basis of some popular iterative techniques.

- ❏ M = diagonal part of A (Jacobi's Method)
- ❏ M = triangular part of A (Gauss-Siedel Method)
- ❏ M = combination of first two (successive over-relaxation).

Some notes on linear system solvers:

- ❏ The L and U factors of a sparse matrix may be dense
- ❏ Direct factorization therefore requires more memory
- ❏ Factorization itself requires n^3 operations for an $n \times n$ matrix.
- ❏ Factorizations are good for smaller systems with a number of right-hand-sides.
- ❏ The core operation of an iterative solver is the application of a matrix on a vector (n^2 complexity).
- ❏ The convergence of an iterative method is dependent on the matrix.
- ❏ Iterative methods are memory efficient (use only as much memory as is required).

Eigenvalues and Eigenvectors:

- ❏ Multiplying a matrix with a vector normally changes the direction of the vector. However, in certain specific directions, the effect of applying the matrix is simply a scaling of the vector.
- ❏ The directions are referred to as the eigenvectors.
- ❏ The scaling factors are the eigenvalues of the matrix.

Computing Eigenvalues:

From definition,

$Ax = rx$ (r is the matrix of eigenvalues at diagonals).

or $(A-rI)x = 0$.

Simple case:

$$A = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Equating *A-rI = 0* yields

$$\begin{bmatrix} 3-r & 0 & 0 \\ 0 & 2-r & 0 \\ 0 & 0 & 0-r \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

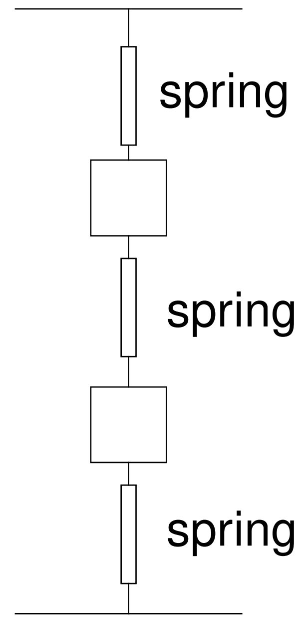
❑ The eigenvalues can be determined by solving the equation *(3-r) (2-r) r = 0*; or *r = 0, 2, 3*.

❑ The polynomial above is referred to as the characteristic polynomial.

❑ The eigenvectors cab be computed by solving *(A-rI)x = 0*. For this particular problem the eigenvectors are (1, 0, 0), (0, 1, 0), and (0, 0, 1).

Why Eigenvalues?

$$\frac{d^2 u}{dt^2} + \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} u = 0$$



- The eigenvalues of the system are 1 and 3 and eigenvectors (1, 1) and (1, -1).

- The solution to the system is simply given by

$u = (a_1 \cos t + b_1 \sin t)\ (1\ 1)^T +$

$(a_2 \cos 1.7t + b_2 \sin 1.7t)\ (1\ -1)^T$

Eigenvalues give fundamental vibration frequencies. Crystal lattices sound familiar (sparse eigenvalue problems)?.