CV5100 – MUDE
Modeling, Uncertainty, and Data for Engineers
Ch4 – Linear Algebra

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Numerical Modelling, Linear Algebra, Optimization

Date	Day	Week	Lecture#	Topic	Topic summary
28-Jul-25	Mon	1			NO CLASS
29-Jul-25	Tue	1			NO CLASS
30-Jul-25	Wed	1	1	Introduction lecture	motivation, course content, logistics, etc.
31-Jul-25	Thu	1	2	Modelling Concepts	sudheendra's part, course logistics; model classification
4-Aug-25	Mon	2	Asst-0		**Software installation & github**
5-Aug-25	Tue	2	3	Numerical Modelling	model decisions, verification vs. validation; differential equations in structural engg, examples, ODE types (linear, nonlinear, order)
6-Aug-25	Wed	2	4	Numerical Modelling	Analytical vs. Numerical solutions, code, algorithm
7-Aug-25	Thu	2	5	Numerical Modelling	Numerical derivative/Finite Differences, Taylor series, error, convergence, forward, backward difference
11-Aug-25	Mon	3	Asst-1		**Finite difference, convergence rate, newton-raphson for finding roots (solving an equation)**
12-Aug-25	Tue	3	6	Numerical Modelling	Central finite diff (1st &2nd order); Numerical integration; IVP example, accuracy/error, convergence,
13-Aug-25	Wed	3	7	Numerical Modelling	stability, explicit vs. implicit; BVP -- e.g. analytical, numerical/FDM, code implementation
14-Aug-25	Thu	3	8	Numerical Modelling	BVP matrix eqn; PDEs - types, gradient and laplacian operators,
18-Aug-25	Mon	4	Asst-2		**IVP & BVP numerical solutions - explicit vs implicit and implementing matrix eq solving using inverse**
19-Aug-25	Tue	4	9	Linear Algebra	Vector spaces, span, linear dependence, basis, dimension, examples, tensor vs. matrix
20-Aug-25	Wed	4	10	Linear Algebra	System of linear eqns, matrix form, solution approach-direct
21-Aug-25	Thu	4	11	Linear Algebra	matrix eqns solutions approach - iterative methods
25-Aug-25	Mon	5	Asst-3		**--**
26-Aug-25	Tue	5	-	Linear Algebra	**NO CLASS**
28-Aug-25	Thu	5	12	Linear Algebra	Eigenvalueproblem, solution approaches, compliexity/scaling; parallel computing?
29-Aug-25	Fri	5	13		Quiz-1 @ 8am
1-Sep-25	Mon	6	Asst-4		**Direct vs Iterative method implementation and comparison; convergence, error plot etc.; Eig vs Eigs**
2-Sep-25	Tue	6	14	Optimization	Classification, Mathematical formulations, standard form, key concepts
3-Sep-25	Wed	6	15	Optimization	Gradient based approaches
4-Sep-25	Thu	6	16	Optimization	Non-gradient approaches
8-Sep-25	Mon	7	Asst-5		
9-Sep-25	Tue	7	17	Uncertainty and Estimation	random variables (rv), covariance, correlation; goodness of fit concepts

Outline

- Vector space concepts
- System of linear equations
- Solution using direct methods
- Solution using indirect (iterative) methods
- Eigenvalue problem
- Orthogonality and orthogonalization

Vector space concepts

- Vector (Linear) space and subspace
- Span
- Linear dependence/independence
- Basis
- Dimension
- Orthogonal vs. non-orthogonal basis
- Column space, null space, rank

System of Linear Equations

- Algebraic to Matrix form

$$
\begin{aligned}
y_1 &= a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n \\
y_2 &= a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n \\
\vdots & \qquad\qquad\qquad \vdots \\
y_m &= a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n
\end{aligned}
\qquad
\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \ldots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}
$$

$$\mathrm{y} = \mathrm{Ax}$$

$$\mathrm{y} = \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} x_1 + \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{bmatrix} x_2 + \cdots + \begin{bmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{bmatrix} x_n$$

- Give an example of linear equation in structural engineering

y is an element of the range space of A: $\mathrm{y} \in \mathcal{R}(\mathrm{A})$

Solution using direct methods

- Gaussian Elimination

Elementary row operations to get row echelon form:
1. Interchanging two rows.
2. Multiplying a row by a non-zero scalar.
3. Adding a scalar multiple of one row to another.

$$\begin{aligned} 2x + y - z &= 8 \qquad (L_1) \\ -3x - y + 2z &= -11 \qquad (L_2) \\ -2x + y + 2z &= -3 \qquad (L_3) \end{aligned}$$

<table>
<tr><th>System of equations</th><th>Row operations</th><th>Augmented matrix</th></tr>
<tr><td>$\begin{aligned} 2x + y - z &= 8 \\ -3x - y + 2z &= -11 \\ -2x + y + 2z &= -3 \end{aligned}$</td><td></td><td>$\left[\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ -3 & -1 & 2 & -11 \\ -2 & 1 & 2 & -3 \end{array}\right]$</td></tr>
<tr><td>$\begin{aligned} 2x + y - z &= 8 \\ \tfrac{1}{2}y + \tfrac{1}{2}z &= 1 \\ 2y + z &= 5 \end{aligned}$</td><td>$L_2 + \tfrac{3}{2}L_1 \to L_2$
$L_3 + L_1 \to L_3$</td><td>$\left[\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & \tfrac{1}{2} & \tfrac{1}{2} & 1 \\ 0 & 2 & 1 & 5 \end{array}\right]$</td></tr>
<tr><td>$\begin{aligned} 2x + y - z &= 8 \\ \tfrac{1}{2}y + \tfrac{1}{2}z &= 1 \\ -z &= 1 \end{aligned}$</td><td>$L_3 + -4L_2 \to L_3$</td><td>$\left[\begin{array}{ccc|c} 2 & 1 & -1 & 8 \\ 0 & \tfrac{1}{2} & \tfrac{1}{2} & 1 \\ 0 & 0 & -1 & 1 \end{array}\right]$</td></tr>
<tr><td>$\begin{aligned} 2x + y &= 7 \\ \tfrac{1}{2}y &= \tfrac{3}{2} \\ -z &= 1 \end{aligned}$</td><td>$L_1 - L_3 \to L_1$
$L_2 + \tfrac{1}{2}L_3 \to L_2$</td><td>$\left[\begin{array}{ccc|c} 2 & 1 & 0 & 7 \\ 0 & \tfrac{1}{2} & 0 & \tfrac{3}{2} \\ 0 & 0 & -1 & 1 \end{array}\right]$</td></tr>
<tr><td>$\begin{aligned} 2x + y &= 7 \\ y &= 3 \\ z &= -1 \end{aligned}$</td><td>$2L_2 \to L_2$
$-L_3 \to L_3$</td><td>$\left[\begin{array}{ccc|c} 2 & 1 & 0 & 7 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & -1 \end{array}\right]$</td></tr>
<tr><td>$\begin{aligned} x &= 2 \\ y &= 3 \\ z &= -1 \end{aligned}$</td><td>$L_1 - L_2 \to L_1$
$\tfrac{1}{2}L_1 \to L_1$</td><td>$\left[\begin{array}{ccc|c} 1 & 0 & 0 & 2 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & -1 \end{array}\right]$</td></tr>
</table>

https://en.wikipedia.org/wiki/Gaussian_elimination

Solution using direct methods

- LU decomposition

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- Decomposes matrix A into:
  - L: Lower triangular matrix
  - U: Upper triangular matrix
- Solves $AX = B$ by solving $LY = B$ and then $UX = Y$.

- Useful for multiple RHS
  e.g.?

- What if A is symmetric?
  LU → LL^T Cholesky

Solution using direct methods

- Gaussian Elimination – Computational efficiency
  - Eliminate elements of first column – nxn ops
  - For every subsequent column reduce n by 1
  - Sum of squares of n natural number – O(n^3)
- Run time scaling
- Memory scaling (storing the matrix); 8 bytes per number in 64-bit (double precision) – 15 decimals
- Triangular matrix – solved sequentially (not efficient for parallel computing)
- Finds the exact solution in a finite number of steps

Eigenvalue problem

- Definition and details
- Computational complexity/scaling
- *eig* vs. *eigs* eigensolvers (numpy vs scipy) – full vs sparse matrices – direct vs indirect/iterative methods
- Inverse and pseudoinverse
- Energy and eigenvalues

- Where do we come across eigenvalues in structural engineering?

Orthogonalization

- Gram-Schmidt process

Given k nonzero linearly-independent vectors $\mathbf{v}_1, \ldots, \mathbf{v}_k$ the Gram–Schmidt process defines the vectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ as follows:

$$
\begin{aligned}
\mathbf{u}_1 &= \mathbf{v}_1, \\
\mathbf{u}_2 &= \mathbf{v}_2 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_2), \\
\mathbf{u}_3 &= \mathbf{v}_3 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_3) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_3), \\
\mathbf{u}_4 &= \mathbf{v}_4 - \mathrm{proj}_{\mathbf{u}_1}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_2}(\mathbf{v}_4) - \mathrm{proj}_{\mathbf{u}_3}(\mathbf{v}_4), \\
&\ \ \vdots \\
\mathbf{u}_k &= \mathbf{v}_k - \sum_{j=1}^{k-1} \mathrm{proj}_{\mathbf{u}_j}(\mathbf{v}_k),
\end{aligned}
$$

The vector projection of a vector $\mathbf{v}$ on a nonzero vector $\mathbf{u}$ is defined

$$\mathrm{proj}_{\mathbf{u}}(\mathbf{v}) = \frac{\langle \mathbf{v}, \mathbf{u} \rangle}{\langle \mathbf{u}, \mathbf{u} \rangle} \mathbf{u}$$

https://en.wikipedia.org/wiki/Gram%E2%80%93Schmidt_process

Solution using indirect methods

- Jacobi iteration

Let $A\mathbf{x} = \mathbf{b}$ be a square system of n linear equations, where:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}.$$

$$\mathbf{A} = \mathbf{D} + \mathbf{R}$$

$$\mathbf{g}(\mathbf{x}) = \mathbf{D}^{-1}(\mathbf{b} - \mathbf{R}\mathbf{x})$$

$$\mathbf{f}(\mathbf{x}) = \mathbf{g}(\mathbf{x}) - \mathbf{x}$$

$$\mathbf{e}(\mathbf{x}) = \mathbf{x} - \mathbf{x}^*$$

$$\mathbf{e}(\mathbf{x}_{k+1}) = \left(\mathbf{I} - \mathbf{D}^{-1}\mathbf{A}\right)\mathbf{e}(\mathbf{x}_k)$$

$$\mathbf{x}_{k+1} = \mathbf{g}(\mathbf{x}_k)$$

$$\|\mathbf{I} - \mathbf{D}^{-1}\mathbf{A}\| < 1$$

$$\mathbf{x}_{k+1} = (1-\omega)\mathbf{x}_k + \omega\mathbf{g}(\mathbf{x}_k)$$

$$\|\mathbf{I} - \omega\mathbf{D}^{-1}\mathbf{A}\| < 1$$

- Fixed-point iteration
- Residual vs. Error
- L^2 norm
- Condition number
- Spectral radius

$$\kappa(A) = \|A\| \cdot \|A^{-1}\|$$

$$\|A\|_2 = \max_{\|x\|_2=1} \|Ax\|_2$$

$$\rho(A) = \max\{|\lambda| : \lambda \text{ is an eigenvalue of } A\}$$

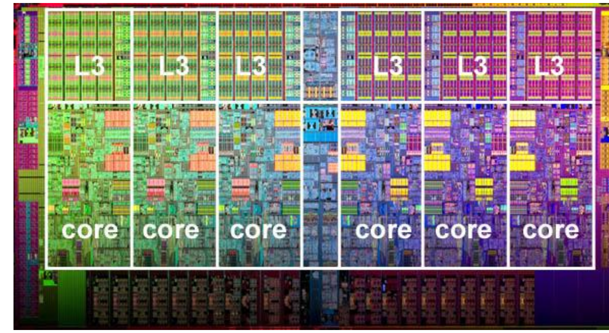
Solution using indirect methods

- Gauss-Seidel Method
- Conjugate Gradient Method
- GMRES
- Preconditioned Conjugate Gradient (PCG)
- Multigrid methods

- Anderson-Jacobi
- Alternating Anderson Jacobi

Pratapa, P. P., Suryanarayana, P., & Pask, J. E. (2016). Anderson acceleration of the Jacobi iterative method: An efficient alternative to Krylov methods for large, sparse linear systems. *Journal of Computational Physics*, *306*, 43-54.

High Performance & Parallel Computing



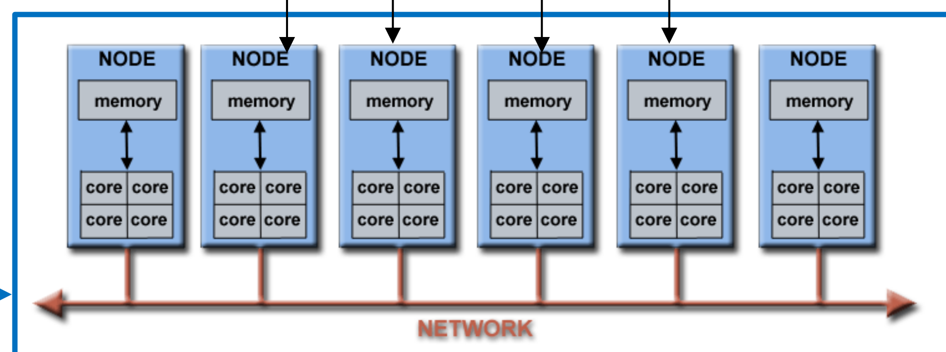
$$b_i = A_{i1}x_1 + A_{i2}x_2 + \ldots + A_{in}x_n = \Sigma_{j=1}^{n} A_{ij}x_j$$

$$\begin{bmatrix} A_{11} & \ldots & A_{1n} \\ A_{21} & \ldots & A_{2n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \ldots & A_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

```
% Given, Matrix A of size n x n.
% Given, Vector x of size n x 1.
% Find, Vector b = A*x.
for i=1:n
    S = 0;
    for j=1:n
        S = S + A(i,j)*x(j);
    end
    b(i) = S;
end
```

Run on multiple computers

Computer Cluster



Ref: https://computing.llnl.gov/tutorials/parallel_comp/

Other things if you are curious

- Scientific/High-performance computing
- Profiling
- BLAS
- LAPACK
- MPI
- PETSc
- Threading
- Parallel scaling, parallel computing
- Cache, retrieval
- Communication
- Petaflops, Exaflops, Supercomputers