Lecture 06 – Algorithms for Linear Algebra

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NERS/ENGR 570 - Methods and Practice of Scientific Computing (F22)

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Outline

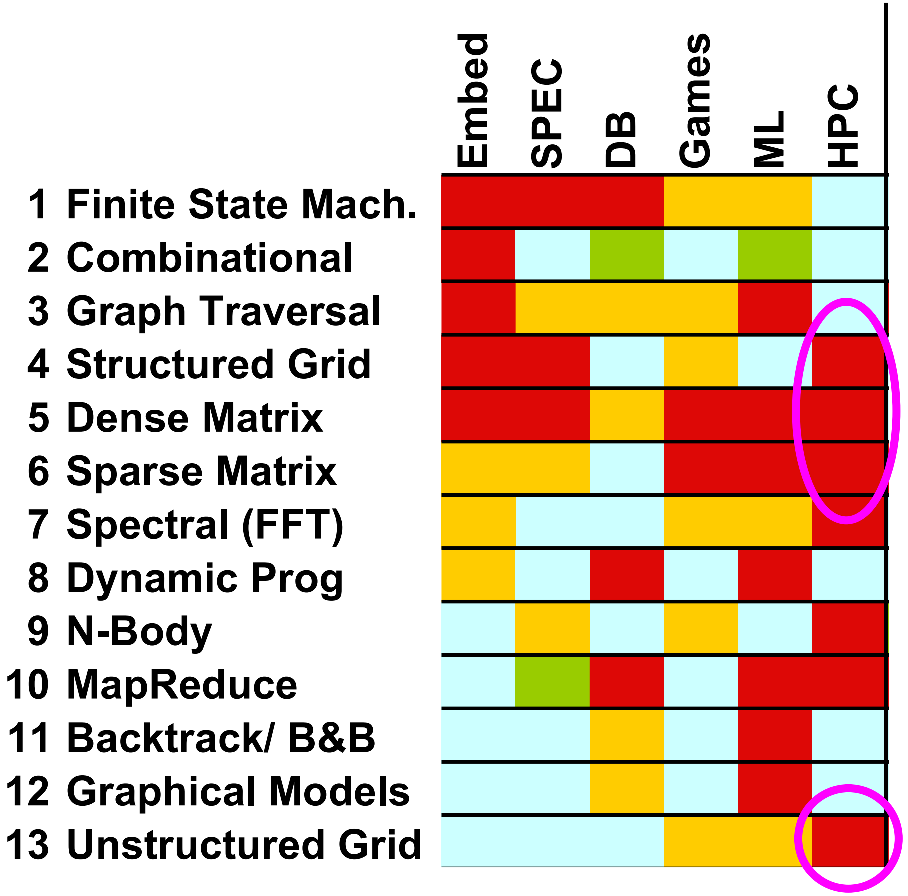
- Recap of our progress so far…
- Linear Algebra Fundamentals
- Dense vs. Sparse Linear Systems
  - Where do they come from?
- Solution of Linear Systems
  - Direct methods and LU Decomposition

Learning Objectives: By the end of Today's Lecture you should be able to

- *(Knowledge)* interpretate meaning of some vector norms
- (*Value/Knowledge*) explain how to think about programming equations in linear algebra
- (*Knowledge*) program the basic kernels needed for linear algebra
- *(Knowledge)* explain the differences of dense and sparse matrix storage formats

Overview

- What types of problems are solved with Linear Algebra?
  - Linear systems of equations
  - Eigenvalue problems
  - Matrix factorizations
  - Overdetermined system of equations
    - Least-Squares (Data fitting)



Linear Algebra Fundamentals

Basics of Linear Systems

$\rightarrow a_{11}x_1 + a_{21}x_2 + \dots + a_{n1}x_n = b_1$

$a_{12}x_1 + a_{22}x_2 + \dots + a_{n,2}x_n = b_2$

$\dots$

$\underline{x} = \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} \quad \underline{b} = \begin{bmatrix} b_1 \\ \vdots \\ \vdots \\ b_m \end{bmatrix}$

$\underline{\underline{A}} = \begin{bmatrix} a_{11} & a_{21} & \dots & a_{n1} \\ a_{12} & a_{22} & \dots & a_{n2} \\ & & & \\ & & & a_{n,m} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$

$\underline{\underline{A}}\,\underline{x} = \underline{b}$

dot product

matrix vector multiplication

$m > n \rightarrow$ over-determined (Tall-Skinny)

$m = n \rightarrow$ square, fully determined

$m > n \rightarrow$ underdetermined (short-wide)

The Residual and Norms

$\underline{\underline{A}}\,\underline{x} = \underline{b}$ $\qquad b - Ax = 0$

$\tilde{x} = x + \varepsilon$ $\qquad b - A\tilde{x} \neq 0 = \text{residual } (\vec{r})$

residual "dual" of the error

$\|r\|$

$\|r\|_1$

$\|r\|_2$

$\|r\|_\infty$

Norms of Vectors

$$\|r\|_1 = |r_1| + |r_2| + \cdots + |r_n| \longrightarrow \text{"total error"}$$

$$\|r\|_2 = \sqrt{r_1^2 + r_2^2 + \cdots + r_n^2} \longrightarrow \text{"average error"}$$

$$\|r\|_\infty = \max(|r_1|, |r_2|, \ldots, |r_n|) \longrightarrow \text{"max. local error"}$$

Mean Sauare Error

$$\|r\|_p = \left(|r_1|^p + |r_2|^p + \cdots + |r_n|^p\right)^{1/p}$$

$$\|r\|_2 = \sqrt{\underline{r}^T \cdot \underline{r}}$$

Going from Chalkboard to Terminal

$$\|r\|_2 = \left(\sum_{i=1}^{n} r_i^2\right)^{1/2} \leftarrow$$

1: Sum variable

2: $\boxed{\text{pow}(v(i), 2)}$ of multiplication

```
nrm2( v(:), n) {
double sum = 0.0;
    for( i=0; i++; i<n) {
        sum += v(i)*v(i)
    }
    return sum;
}
```

Types of Linear Algebra Operations

BLAS

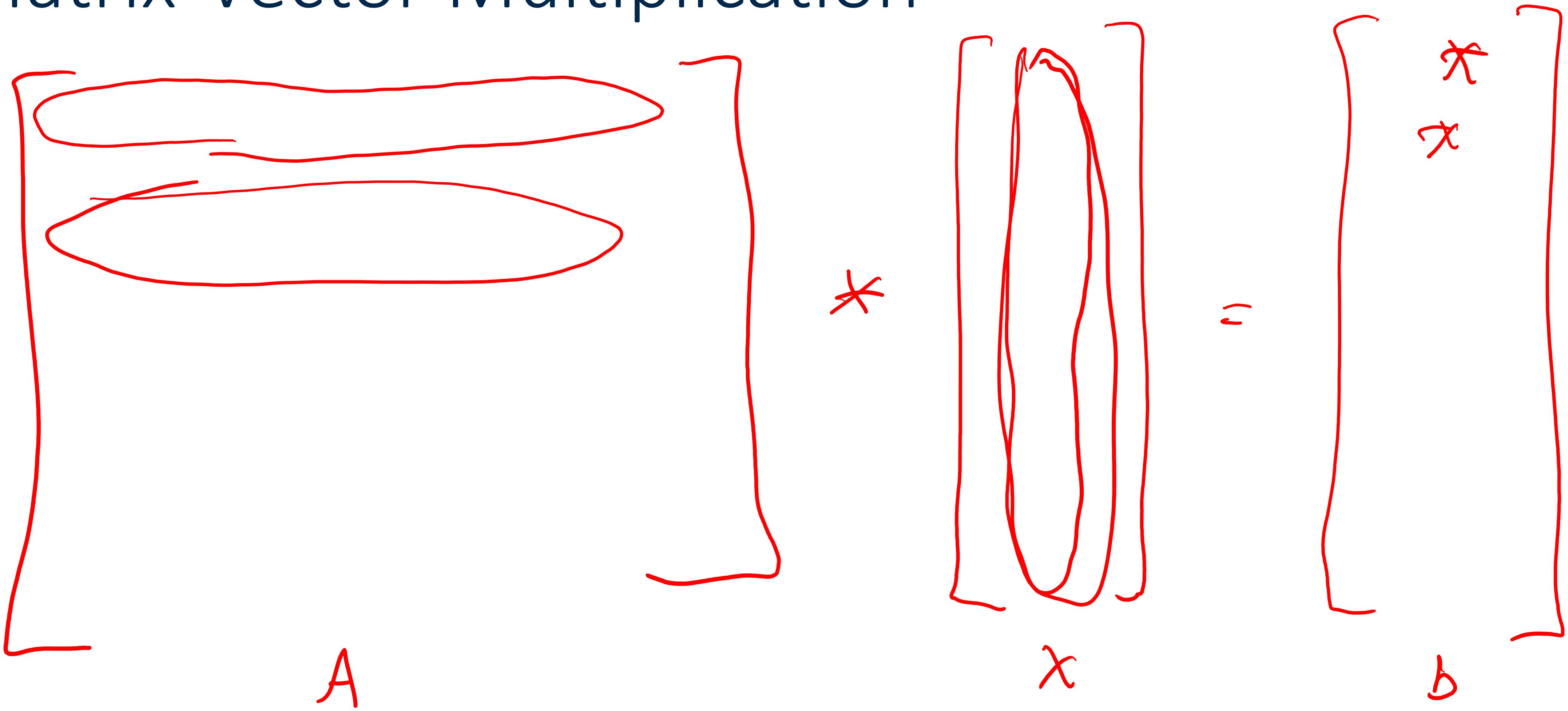
~~scalar-scalar: 0 loops~~

scalar-vector: 1 loop
vector-vector: 1 loop } Level 1

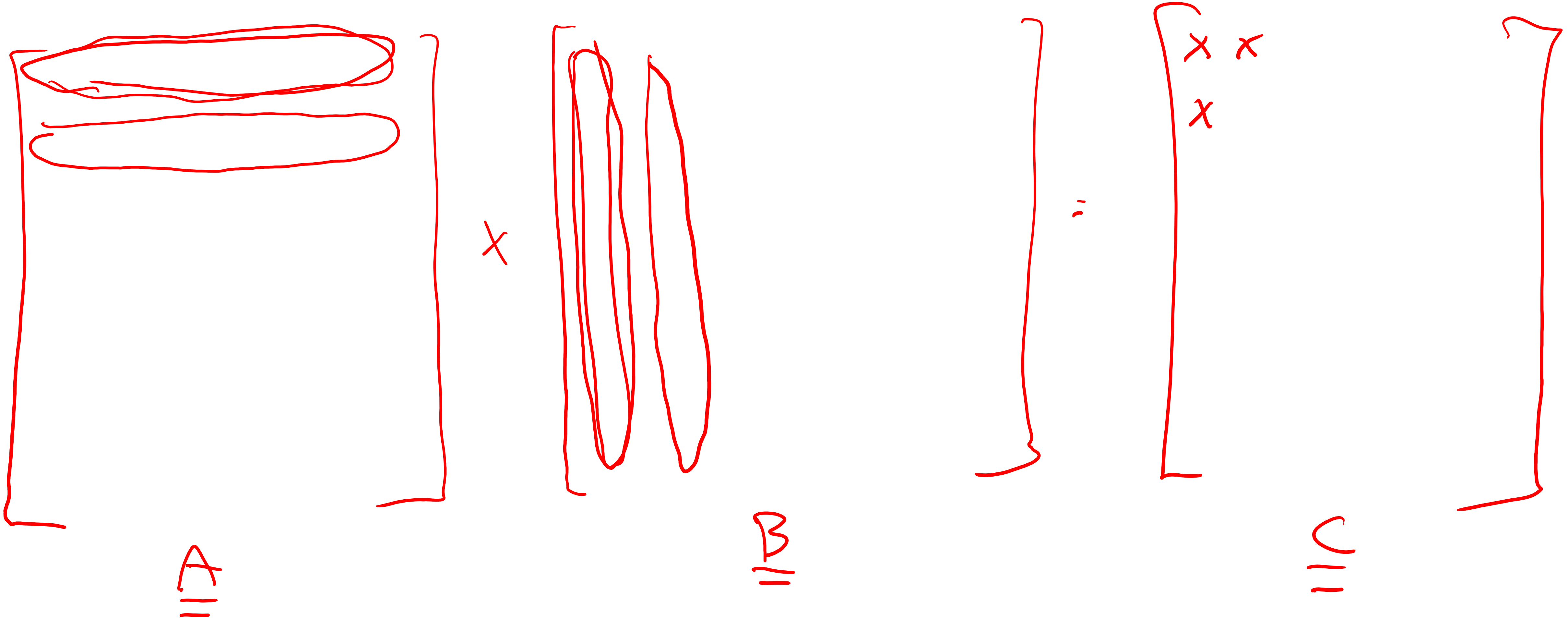
Matrix-vector: 2 loops
scalar-Matrix: 2 loops } Level 2

Matrix-Matrix: 3 loops } level 3

Matrix-Vector Multiplication



Matrix-Matrix Multiplication



Complexity and Cost of Solving Linear Systems

$O(n^3)$ for direct methods → $n^{2.376}$

Historically, what's a big N

1950's: N = 20 ~ 6 hours

1965: N = 200

1980: N = 2,000

1995: N = 20,000

2010: N = 200,000

(4 GB)

10^4

MFLOPS 10^6

GFLOPS 10^{12}

TFLOPS

PFLOPS

EFLOPS 10^{18}

$\frac{12}{4} = 3$

$O(n^3)$ → # of operations "classical view" ⟹ # operations + data movement

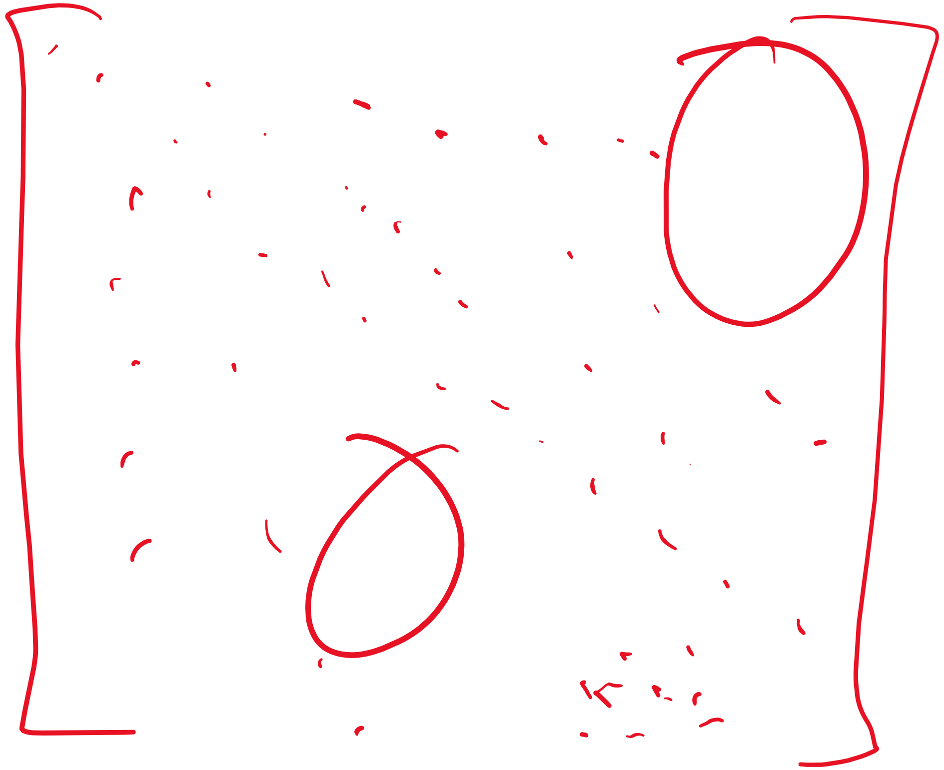
Dense vs. Sparse Linear Algebra

What are Dense and Sparse Linear Systems

Dense

Mostly nonzer

Sparse



fill in usually < 20%

How do dense linear systems arise?

photos, pictures,

$X^T X$

$= \begin{bmatrix} x & x & x \\ x & x & x \\ x & x & \end{bmatrix}$

Integral Methods

- the solution at any point is a function of the solution at all points

Boundary Integral Equations

$\nabla^2 u(x) = 0$ domain

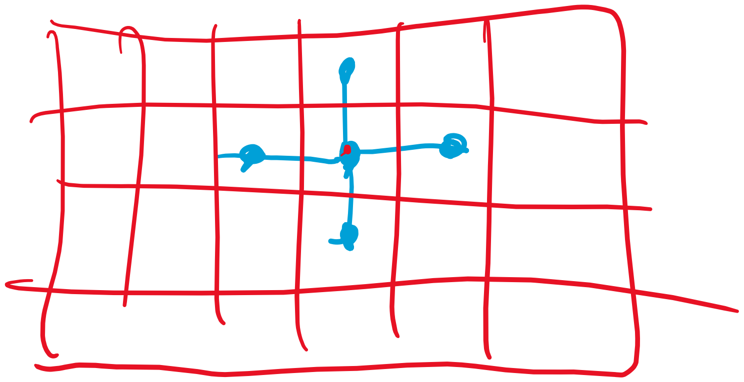
$u(x) = f(x)$ boundary

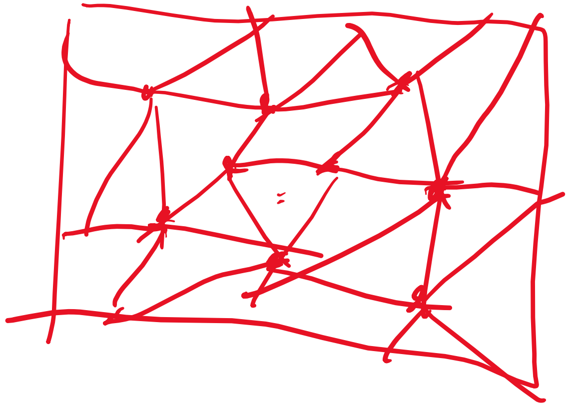
$\longrightarrow u(x) = \int_{\text{boundary}} G(x, s) f(s) \, ds$

How do sparse linear systems arise?

Discretize PDE

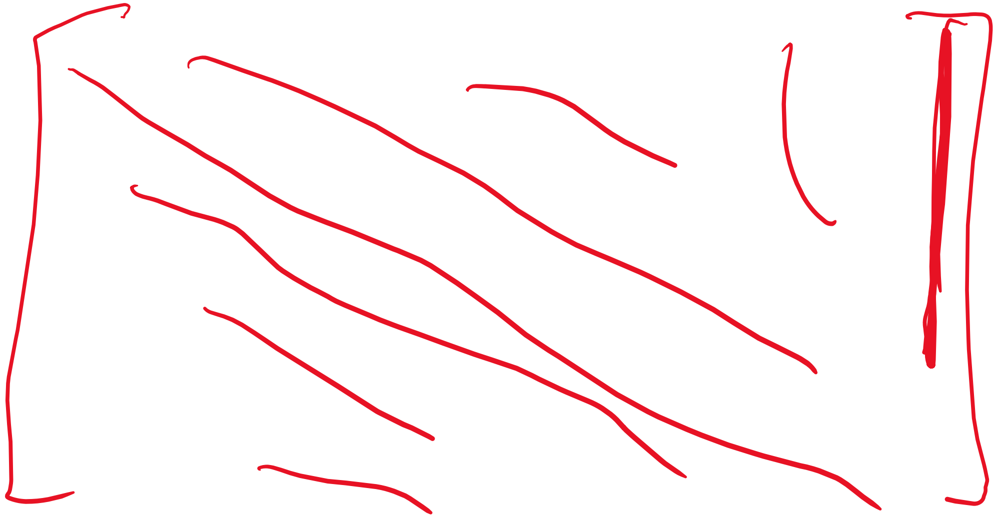
- Finite Difference
- Finite element
- Finite volume





$\nabla^2 u(x) = 0$ domain

$u(x) = f(x)$ boundary



Types of Matrices and Storage Formats

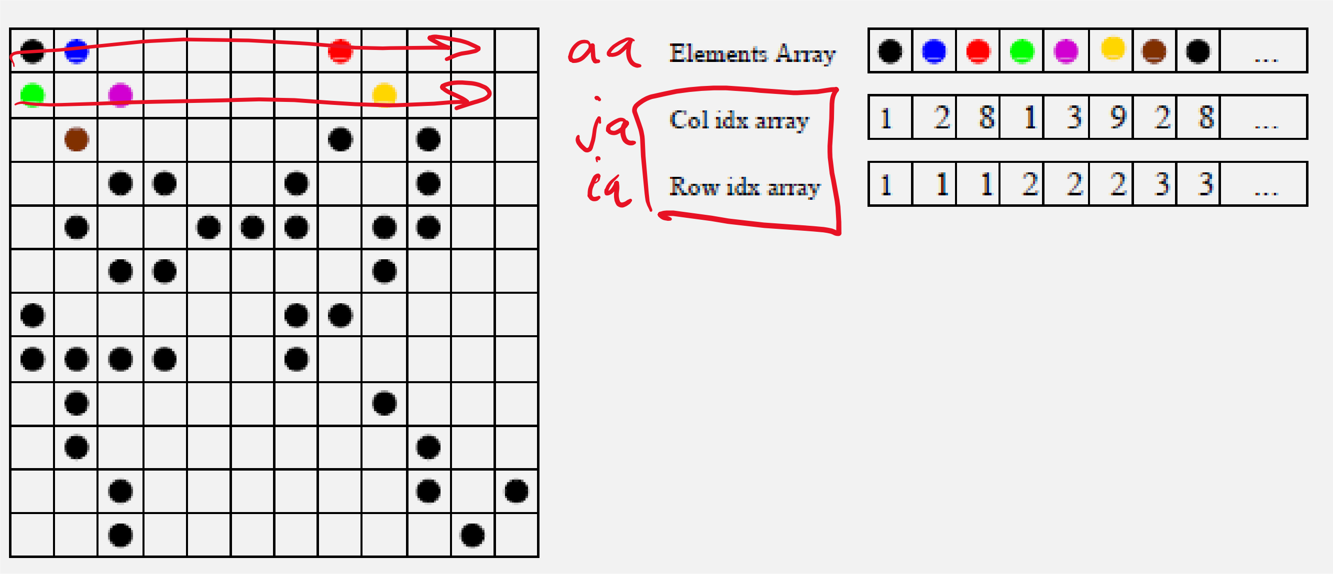
Matrices

symmetric
orthogonal
Triangular / upper or lower
Banded
invertible
positive definite
singular
unitary
orthonormal

Formats

banded
symmetric
coordinate
compressed sparse row

Example: Coordinate (COO) Format



} value

} 2 integer arrays

size nz

nnz

```
do n=1, nnz
   i = ia(n)
   j = ja(n)
   y(i) = y(i) + aa(n)*x(j)
enddo
```

Solving Linear Systems

Overview of Solution Methods

LU Factorization

LU Factorization for Solving Linear Systems

LU: Forward Elimination

LU: Backward Substitution

Fast LU Factorizations