MASTER IN ENTREPRENEURSHIP INNOVATION MANAGEMENT
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DIGITAL TECH

High Performance Computing

Lesson 1: Basic scientific computing tools

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Lesson 1: Basic scientific computing tools

1. Vectors (arrays)
2. Matrices
3. Linear systems

Vectors: preliminaries

Different perspective:

- Physics: length, direction (pointing from A to B) $\quad v \quad \longrightarrow$
- Mathematician: couple (ordered pairs, tuples) of coordinates between commas

$$v = (v_1, v_2) \qquad \textit{couple,} \qquad \textit{two-dimensional vector}$$

$$w = (w_1, w_2, \ldots, w_t) \qquad \textit{tuple,} \qquad \textit{t-dimensional vector}$$

- Computer science: list of numbers. Row and column vectors

$$w = [5,\ 3,\ 6,\ -4,\ \pi] \qquad v = \begin{bmatrix} 6 \\ 2 \\ 4 \end{bmatrix}$$

$v_1, v_2, \ldots$ are called components

Vectors: preliminaries (2)

Let be $v = [v_1, v_2, \ldots, v_n]$ $\quad w = [w_1, w_2, \ldots, w_n]$ vectors and $k \in \mathbf{R}$ a real number (scalar)

- norm (length) $\quad \|v\| = \sqrt{v_1^2 + v_2^2 + \cdots + v_n^2}$
- sum $\quad v + w = [v_1 + w_1, v_2 + w_2, \ldots, v_n + w_n]$
- inner (standard, scalar) product $\quad v \cdot w = v_1 \cdot w_1 + v_2 \cdot w_2 + \cdots + v_n \cdot w_n$
  (please note: the result is a number).
- $kv = k \cdot v = [kv_1, kv_2, \ldots, kv_n]$ is the scalar multiplication.
  (please note: the result is a vector). The resulting vector is k times as long as v (k times the original length
- Pointwise (Hadamard) product $v \circ w = [v_1 \cdot w_1, v_2 \cdot w_2, \ldots, v_n \cdot w_n]$

Vectors: preliminaries (3)

- if $\|v\| = 1$ then v is called **Unit vector**

- vector $\mathbf{0} = [0, 0, , \ldots, 0]$ is called **Zero vector**. Is the **neutral element** for the additive operation.

  It is the unique vector of norm zero.

- $z = -v = \left[-v_1, -v_2, \ldots, -v_n \right]$ is the **opposite vector** of v. Indeed $v + z = v + (-v) = \mathbf{0}$.

- the **angle** between vectors $v, w \neq \mathbf{0}$ is given by $\Theta_{v,w} = arccos \dfrac{v \cdot w}{\|v\| \cdot \|w\|}$

- note that if $v \cdot w = 0$ vectors are called **orthogonal (perpendicular, normal)**

- if $v \neq \mathbf{0}$ the vector $w = v/\|v\|$ is a unit vector

Vectors: preliminaries (4)

- $V = V_n = \{[v_1, v_2, \ldots, v_n] \mid v_i \in R\}$ is the (real) linear space of dimension n.

- **a linear combination** of k elements of V is of the form

$$a_1 v_1 + a_2 v_2 + \cdots + a_k v_k$$

  where $a_1, \ldots, a_k$ are scalar and $v_1, \ldots, v_k$ are vectors of V
  Scalars are also called the **coefficients of the linear combination.**

- Vectors $S = \{v_1, v_2, \ldots, v_k\}$ are said linearly independent, if no element of S can be written as a linear combination of the other elements of S.

- a basis B of V_n is a linearly independent set B of size n

- standard basis is

$$e_1 = [1, 0, 0, \ldots, 0, 0], \quad e_2 = [0, 1, 0, \ldots, 0, 0], \quad \ldots \quad e_n = [0, 0, 0, \ldots, 0, 1]$$

Vectors: preliminaries (5)

(i) $v \cdot v = |v|^2$;

(ii) $v \cdot w = w \cdot v$;

(iii) $v \cdot (w + z) = v \cdot w + v \cdot z$;

(iv) $v \cdot (\alpha w) = (\alpha v) \cdot w = \alpha(v \cdot w)$;

(v) $|v \cdot w| \leq |v||w|$; ← Cauchy-Schwartz inequality

(vi) $|v + w| \leq |v| + |w|$; ← Triangle inequality

Lesson 1: Basic scientific computing tools

1. Vectors (arrays)
2. Matrices
3. Linear systems

Matrices: main concepts

- A matrix $A \in R^{m \times n}$ is a two-dimensional table in two big (round or square) brackets with m rows and n columns

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{bmatrix}.$$

  - A is a rectangular/square array of numbers, arranged in rows and columns.
  - $m \times n$ is the order of the matrix

- Please note:
  - row vectors are matrices with $m = 1$ of order $1 \times n$
  - column vectors are matrices with $n = 1$ of order $m \times 1$

Matrices: main concepts

- Matrices are usually denoted by capital letters

  (example) Matrix $C = \begin{bmatrix} 1 & 2 & -3 \\ 3 & 4 & 0 \end{bmatrix}$ is a 2×3 matrix.

- A is also denoted as

$$A = (a_{i,j})$$

  where real number $a_{i,j}$ is called **entry** or **element** with row index i and column index j

- A matrix with $m = n$ is called **square matrix** of order n

  A matrix with $m \neq n$ is called **rectangular matrix**

Matrices: main concepts

A matrix A of order $m \times n$ contains

- m rows usually denoted by

$$A_1, A_2, \ldots, A_m$$

- n columns usually denoted by

$$A^1, A^2, \ldots, A^n$$

- main diagonal is given by

$$(a_{1,1}, a_{2,2}, \ldots)$$

$$A = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{bmatrix}$$

$$A \equiv \left(\begin{array}{c} A_1 \\ \hline A_2 \\ \hline \ldots \\ \hline A_m \end{array} \right) \qquad A \equiv (A^1 | A^2 | \ldots | A^n)$$

Matrices: main concepts

The set $R^{m,n} = \mathcal{M}_{m,n}(R)$ of all matrices of order $m \times n$ is a linear space with two binary operations: **sum** and **scalar multiplication**.

- The **sum** $C = A + B$ of two matrices is allowed only if they share the order (same number of rows and columns). It holds

$$c_{i,j} = a_{i,j} + b_{i,j}, \qquad \forall\, i = 1, \dots, m, \quad j = 1, \dots, n$$

  That is

$$C = A + B = (a_{ij}) + (b_{ij}) = (a_{ij} + b_{ij})\,.$$

- If A is a matrix and $\alpha \in R$ is a scalar **scalar multiplication**, matrix $C = \alpha \cdot A$ is a matrix of the same order of A with entries

$$C = \alpha \cdot A = \alpha \cdot (a_{ij}) = (\alpha a_{ij})\,.$$

Matrices: main concepts

Example

$$\text{Given} \quad A = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 4 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 2 \\ 1 & -2 \\ 3 & -2 \end{pmatrix} \quad \text{compute} \quad C = A + B, \quad D = 6 \cdot A$$

- Sum

$$C = A+B = \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 4 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 2 \\ 1 & -2 \\ 3 & -2 \end{pmatrix} = \begin{pmatrix} 1+0 & 2+2 \\ 3+1 & 1-2 \\ 4+3 & 1-2 \end{pmatrix} = \begin{pmatrix} 1 & 4 \\ 4 & -1 \\ 7 & -1 \end{pmatrix}$$

- scalar multiplication

$$D = 6 \cdot A = 6 \cdot \begin{pmatrix} 1 & 2 \\ 3 & 1 \\ 4 & 1 \end{pmatrix} = \begin{pmatrix} 6 \cdot 1 & 6 \cdot 2 \\ 6 \cdot 3 & 6 \cdot 1 \\ 6 \cdot 4 & 6 \cdot 1 \end{pmatrix} = \begin{pmatrix} 6 & 12 \\ 18 & 6 \\ 24 & 6 \end{pmatrix}.$$

Matrices: main concepts

- matrix $\mathbf{0} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix}$ is called **zero matrix** or **null matrix**.

It is the **neutral element** for the additive operation. It holds $\mathbf{0} + A = A + \mathbf{0} = A, \quad \forall A \in^{m,n}$.

- Matrix $B = (-a_{ij})$ is the opposite matrix of A

- Difference of two matrices $A - B$ is just sum of A and the the opposite of B

$$A - B = A + (-B) = (a_{ij} - b_{ij}).$$

$$A = \begin{pmatrix} 1 & 1 \\ 2 & 0 \\ 3 & 5 \end{pmatrix} \quad A^T = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 0 & 5 \end{pmatrix}$$

- matrix $A^T = (a_{j,i})$ where rows and columns swap roles is called **transpose** of A

Matrices: main concepts

Structured matrices whose elements values depend od row and column indices

- A is **symmetric** if $a_{ij} = a_{ji}$ $\qquad A = \begin{pmatrix} 1 & 3 & 4 \\ 3 & 1 & 5 \\ 4 & 5 & 2 \end{pmatrix}$

- A is **anti-symmetric** or **skew-symmetric** if $a_{ij} = -a_{ji}$ $\qquad A = \begin{pmatrix} 0 & -3 & -1 \\ 3 & 0 & 5 \\ 1 & -5 & 0 \end{pmatrix}$

- A is **diagonal** if $a_{ij} = 0, \quad \forall\, i \neq j$ $\qquad A = \begin{pmatrix} d_1 & 0 & \dots & 0 \\ 0 & d_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & d_n \end{pmatrix}$

Matrices: main concepts

- $A = I$ is the **identity matrix** if it is a diagonal matrix with $a_{ij} = 1 \quad \forall\, i = j$ $\qquad I_n = \begin{pmatrix} 1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 1 \end{pmatrix}$

- $A = U$ is upper triangular if $a_{ij} = 0 \quad \forall\, i > j$ $\qquad U = \begin{pmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & u_{nn} \end{pmatrix}$

- $A = L$ is lower triangular if $a_{ij} = 0 \quad \forall\, i < j$ $\qquad L = \begin{pmatrix} l_{11} & 0 & \dots & 0 \\ l_{21} & l_{22} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{pmatrix}$

Matrices: multiplication

$$\begin{pmatrix} b_{1,1} & \vdots & b_{1,j} & \vdots & b_{1,p} \\ b_{2,1} & \vdots & b_{2,j} & \vdots & b_{2,p} \\ \vdots & \vdots & \vdots & \vdots & \dots \\ b_{n,1} & \vdots & b_{n,j} & \vdots & b_{n,p} \end{pmatrix} \quad B \quad \text{order } n \times p$$

$$\begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ \dots & \dots & \dots & \dots \\ a_{i,1} & a_{i,2} & \dots & a_{i,n} \\ \dots & \dots & \dots & \dots \\ a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{pmatrix} \qquad c_{ij}$$

A order $m \times n$

matrix multiplication (matrix-matrix product) is a matrix C of order $m \times p$ whose entries are obtained as the dot product of A_i and B^j, that is

$$C = (c_{ij}) = (A_i \cdot B^j), \quad \forall\, i = 1, \dots, m. \quad j = 1, \dots, p$$

Matrices: multiplication

$$\begin{pmatrix} \boxed{b_{1,1}} & \vdots & b_{1,j} & \vdots & b_{1,p} \\ b_{2,1} & \vdots & b_{2,j} & \vdots & b_{2,p} \\ \vdots & \vdots & \vdots & \vdots & \dots \\ b_{n,1} & \vdots & b_{n,j} & \vdots & b_{n,p} \end{pmatrix} \quad B \quad \text{order } n \times p$$

$$\begin{pmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,n} \\ \dots & \dots & \dots & \dots \\ a_{i,1} & a_{i,2} & \dots & a_{i,n} \\ \dots & \dots & \dots & \dots \\ a_{m,1} & a_{m,2} & \dots & a_{m,n} \end{pmatrix}$$

$A \quad \text{order } m \times n$

$$C = A \cdot B = \begin{pmatrix} \boxed{A_1 \cdot B^1} & A_1 \cdot B^2 & \dots & A_1 \cdot B^p \\ A_2 \cdot B^1 & A_2 \cdot B^2 & \dots & A_2 \cdot B^p \\ \vdots & \vdots & \ddots & \vdots \\ A_m \cdot B^1 & A_m \cdot B^2 & \dots & A_m \cdot B^p \end{pmatrix}$$

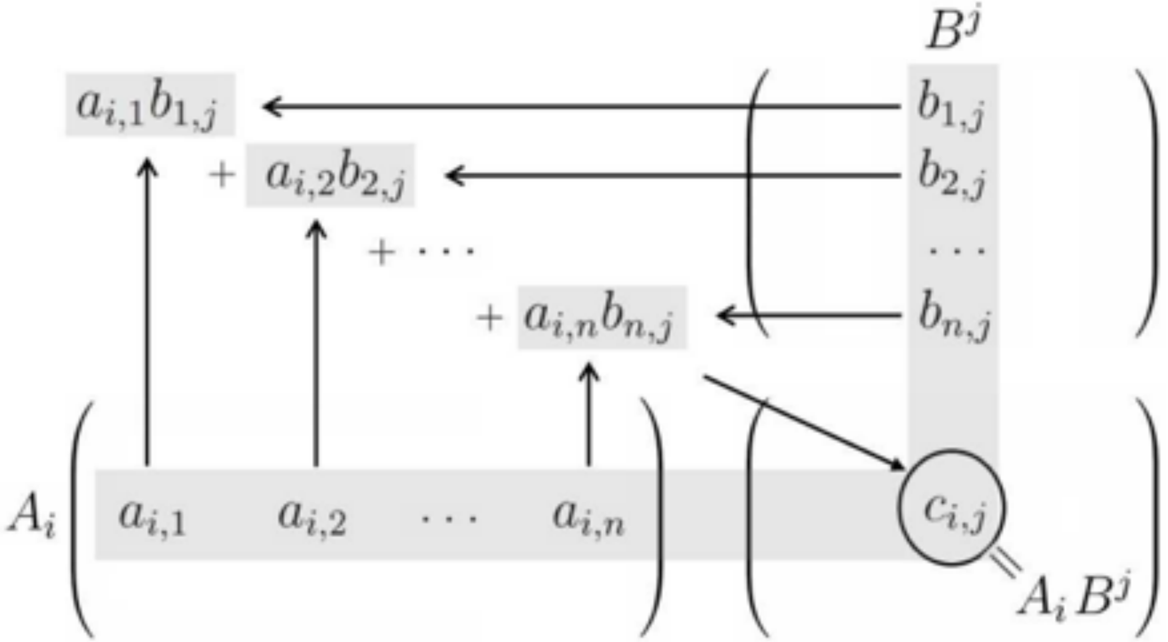
matrix multiplication (matrix-matrix product) is a matrix C of order $m \times p$ whose entries are obtained as the dot product of A_i and B^j, that is

$$C = (c_{ij}) = (A_i \cdot B^j), \quad \forall\, i = 1, \dots, m. \quad j = 1, \dots, p$$

Matrices: multiplication

$$\begin{array}{cc} B^1 & B^2 \end{array}$$
$$B = \begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 4 \end{bmatrix}$$

$$\begin{array}{c} A_1 \\ A_2 \\ A_3 \end{array} \underbrace{\begin{bmatrix} 1 & 2 & 2 \\ 3 & 4 & 0 \\ 5 & -6 & 1 \end{bmatrix}}_{A} \quad \underbrace{\begin{bmatrix} A_1B^1 & A_1B^2 \\ A_2B^1 & A_2B^2 \\ A_3B^1 & A_3B^2 \end{bmatrix}}_{C}$$



Matrices: multiplication

$$
\begin{array}{c} \\ \end{array}
\begin{array}{cc} B^1 & B^2 \end{array}
$$

$$
\underbrace{\begin{bmatrix} 1 & 2 \\ 0 & 1 \\ 1 & 4 \end{bmatrix}}_{B}
$$

$$
\begin{array}{c} A_1 \\ A_2 \\ A_3 \end{array}
\underbrace{\begin{bmatrix} 1 & 2 & 2 \\ 3 & 4 & 0 \\ 5 & -6 & 1 \end{bmatrix}}_{A}
\underbrace{\begin{bmatrix} A_1B^1 & A_1B^2 \\ A_2B^1 & A_2B^2 \\ A_3B^1 & A_3B^2 \end{bmatrix}}_{C}
=
\underbrace{\begin{bmatrix} 3 & 12 \\ 3 & 10 \\ 6 & 8 \end{bmatrix}}_{C}
$$

$$c_{1,1} = A_1 \cdot B^1 = \underbrace{\begin{bmatrix} 1 & 2 & 2 \end{bmatrix}}_{A_1} \cdot \underbrace{\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}}_{B^1} = 1 \cdot 1 + 2 \cdot 0 + 2 \cdot 1 = 3,$$

$$c_{1,2} = A_1 \cdot B^2 = \underbrace{\begin{bmatrix} 1 & 2 & 2 \end{bmatrix}}_{A_1} \cdot \underbrace{\begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix}}_{B^2} = 1 \cdot 2 + 2 \cdot 1 + 2 \cdot 4 = 12.$$

$$c_{2,1} = A_2 \cdot B^1 = \underbrace{\begin{bmatrix} 3 & 4 & 0 \end{bmatrix}}_{A_2} \cdot \underbrace{\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}}_{B^1} = 3 \cdot 1 + 4 \cdot 0 + 0 \cdot 1 = 3,$$

$$c_{2,2} = A_2 \cdot B^2 = \underbrace{\begin{bmatrix} 3 & 4 & 0 \end{bmatrix}}_{A_2} \cdot \underbrace{\begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix}}_{B^2} = 3 \cdot 2 + 4 \cdot 1 + 0 \cdot 4 = 10.$$

$$c_{3,1} = A_3 \cdot B^1 = \underbrace{\begin{bmatrix} 5 & -6 & 1 \end{bmatrix}}_{A_3} \cdot \underbrace{\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}}_{B^1} = 5 \cdot 1 - 6 \cdot 0 + 1 \cdot 1 = 6,$$

$$c_{3,2} = A_3 \cdot B^2 = \underbrace{\begin{bmatrix} 5 & -6 & 1 \end{bmatrix}}_{A_3} \cdot \underbrace{\begin{bmatrix} 2 \\ 1 \\ 4 \end{bmatrix}}_{B^2} = 5 \cdot 2 - 6 \cdot 1 + 1 \cdot 4 = 8.$$

Matrices: multiplication (properties)

(i) **Associativity** $A \in^{m,n}$, $B \in^{n,p}$, $C \in^{p,q}$ then $(AB)C = A(BC)$.

(ii) **Left distributivity** $A \in^{m,n}$, $B, C \in^{n,p}$ then $A(B+C) = AB + AC$.

(iii) **Right distributivity** $A \in^{n,p}$, $B, C \in^{m,n}$. then $(B+C)A = BA + CA$.

(iv) $A \in^{m,n}$, $B \in^{n,p}$, $\alpha \in$ then $\alpha(AB) = (\alpha A)B = A(\alpha B)$.

(v) **Neutral element** I_n and I_m identity matrices (of order n and m), $A \in^{m,n}$ then $I_m A = A I_n = A$

(vi) **Transpose multiplication** $A \in^{m,n}$ and $B \in^{n,p} \implies (AB)^T = B^T A^T$.

Matrices: matrix-vector multiplication as a linear combination

Matrix A by column vector x produces a column Ax that is the linear combination of columns of A with components of x as coefficients

$$\left(A^1 \middle| A^2 \middle| \cdots \middle| A^k\right) \begin{pmatrix} x_1 \\ \hline x_2 \\ \hline \cdots \\ \hline x_k \end{pmatrix} = x_1 \left(A^1 \right) + x_2 \left(A^2 \right) + \cdots + x_k \left(A^k \right)$$

$$A \qquad x \qquad = \qquad x_1 A^1 + x_2 A^2 + \cdots + x_k A^k$$

$$A = \begin{pmatrix} 1 & 4 & \sqrt{3} \\ 3 & 1 & 19 \end{pmatrix}, \quad x = \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix}$$

$$Ax = \begin{pmatrix} 1 & 4 & \sqrt{3} \\ 3 & 1 & 19 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 6 \\ 7 \end{pmatrix}$$

$$= 2 \cdot \begin{pmatrix} 1 \\ 3 \end{pmatrix} + 1 \cdot \begin{pmatrix} 4 \\ 1 \end{pmatrix} + 0 \cdot \begin{pmatrix} \sqrt{3} \\ 19 \end{pmatrix}$$

$$= \quad x_1 A^1 \quad + \quad x_2 A^2 \quad + \quad x_3 A^3$$

Matrices: vector – matrix multiplication as a linear combination

Row vector x by matrix A produces a row xA that is the linear combination of rows of A with components of x as coefficients

$$\left(x_1 \middle| x_2 \middle| \cdots \middle| x_k\right) \left(\begin{array}{c} A_1 \\ \hline A_2 \\ \hline \cdots \\ \hline A_k \end{array}\right) = \begin{array}{l} \, x_1 \left(\quad A_1 \quad \right) \\ + \, x_2 \left(\quad A_2 \quad \right) \\ \qquad \quad \cdots \\ + \, x_k \left(\quad A_k \quad \right) \end{array}$$

$$x \qquad\qquad A \quad = x_1 A_1 + x_2 A_2 + \cdots + x_k A_k$$

$$xA = \begin{array}{c} x \\ \begin{pmatrix} 1 & 2 & 0 \end{pmatrix} \end{array} \cdot \begin{array}{c} A \\ \begin{pmatrix} 1 & 0 & 5 & 2 \\ 1 & 4 & 4 & 0 \\ 5 & 5 & 2 & 3 \end{pmatrix} \end{array} =$$

$$= \begin{pmatrix} 3 & 8 & 13 & 2 \end{pmatrix}$$

$$= \begin{array}{l} \, 1 \cdot (1 \quad 0 \quad 5 \quad 2) \\ + \\ \, 2 \cdot (1 \quad 4 \quad 4 \quad 0) \\ + \\ \, 0 \cdot (5 \quad 5 \quad 2 \quad 3) \end{array} = \begin{array}{c} x_1 A_1 \\ + \\ x_2 A_2 \\ + \\ x_3 A_3. \end{array}$$

Matrices: inverse matrix

- A square matrix of order n. $B = A^{-1}$ is called inverse of A if $BA = AB = I_n$.
- inverse is denoted by $inv(A)$ Alert: not all matrices have an inverse
- matrix

  $A = (a_{ij})$ of order 2 is invertible iff $a_{11}a_{22} - a_{12}a_{21} \neq 0$. In this case it is

$$A^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

$$A = \begin{bmatrix} 9 & -4 \\ 3 & 2 \end{bmatrix} \qquad a_{11}a_{22} - a_{12}a_{21} = 9 \cdot 2 - (-4) \cdot 3 = 30 \neq 0.$$

$$A^{-1} = \frac{1}{9 \cdot 2 - (-4) \cdot 3} \begin{bmatrix} 2 & 4 \\ -3 & 9 \end{bmatrix} = \frac{1}{30} \begin{bmatrix} 2 & 4 \\ -3 & 9 \end{bmatrix} = \begin{bmatrix} \frac{1}{15} & \frac{2}{15} \\ -\frac{1}{10} & \frac{3}{10} \end{bmatrix}$$

Matrices: inverse matrix (properties)

(i) if A^{-1} is the inverse of A, then A is the inverse of A^{-1}.

(ii) If A and B are invertible AB is also invertible and $(AB)^{-1} = B^{-1}A^{-1}$

(iii) If A is invertible then also A^T is invertible and $(A^T)^{-1} = (A^{-1})^T$

(iv) if $A = diag(d_1, d_2, \ldots, d_n)$ is diagonal, then it is invertibile iff $d_1, d_2, \ldots, d_n \neq 0$.

In this case $A^{-1} = diag(d_1^{-1}, d_2^{-1}, \ldots, d_n^{-1})$.

$$\boxed{A = \begin{pmatrix} \frac{3}{2} & 0 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & \frac{4}{\pi} & 0 \\ 0 & 0 & 0 & \frac{e}{3} \end{pmatrix} \qquad A^{-1} = \begin{pmatrix} \frac{2}{3} & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & \frac{\pi}{4} & 0 \\ 0 & 0 & 0 & \frac{3}{e} \end{pmatrix}}$$

Matrices: determinant (small order n=1, n=2, n=3)

Symbols $\quad \det(A), \quad \det A, \quad |A|.$

Case $\quad n = 1, \quad A = (a_{11}) \Rightarrow \det A \overset{\text{def}}{=} a_{11}.$

Case $\quad n = 2, \; A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \Rightarrow \det A \overset{\text{def}}{=} a_{11}a_{22} - a_{12}a_{21}.$

$$\begin{array}{ccccc} & A & & A^1 & A^2 \\ + & + & + & & \end{array} \qquad \begin{array}{ccccc} & A & & A^1 & A^2 \\ & & - & - & - \end{array}$$

$$\begin{bmatrix} \boxed{a_{11}} & \boxed{a_{12}} & \boxed{a_{13}} & a_{11} & a_{12} \\ a_{21} & \boxed{a_{22}} & \boxed{a_{23}} & \boxed{a_{21}} & a_{22} \\ a_{31} & a_{32} & \boxed{a_{33}} & \boxed{a_{31}} & \boxed{a_{32}} \end{bmatrix} \qquad \begin{bmatrix} a_{11} & a_{12} & \boxed{a_{13}} & \boxed{a_{11}} & \boxed{a_{12}} \\ a_{21} & \boxed{a_{22}} & \boxed{a_{23}} & \boxed{a_{21}} & a_{22} \\ \boxed{a_{31}} & \boxed{a_{32}} & \boxed{a_{33}} & a_{31} & a_{32} \end{bmatrix}$$

Case $\quad n = 3 \quad \det A \overset{\text{def}}{=} a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{13}a_{22}a_{31} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33}$

Matrices: determinant (Laplace expansion, recursive definition)

Consider submatrices obtained by rembing 1 row and 1 column

$$A_{ij} = \begin{pmatrix} a_{1,1} & \dots & a_{1,j-1} & * & a_{1,j+1} & \dots & a_{1,n} \\ \dots & \dots & \dots & * & \dots & \dots & \dots \\ a_{i-1,1} & \dots & a_{i-1,j-1} & * & a_{i-1,j+1} & \dots & a_{i-1,n} \\ * & * & * & * & * & * & * \\ a_{i+1,1} & \dots & a_{i+1,j-1} & * & a_{i+1,j+1} & \dots & a_{i+1,n} \\ \dots & \dots & \dots & * & \dots & \dots & \dots \\ a_{n,1} & \dots & a_{n,j-1} & * & a_{n,j+1} & \dots & a_{n,n} \end{pmatrix}$$

$$\det A \stackrel{\text{def}}{=} a_{i1}C_{i1} + a_{i1}C_{i2} + \cdots + a_{in}C_{in} = \sum_{j=1}^{n} a_{ij}C_{ij}.$$

or

$$\det A \stackrel{\text{def}}{=} a_{1j}C_{1j} + a_{1j}C_{2j} + \cdots + a_{nj}C_{nj} = \sum_{i=1}^{n} a_{ij}C_{ij}.$$

where

$$C_{ij} = (-1)^{i+j} \det A_{ij}.$$

Matrices: determinant (properties)

$A = (A^1 | \, A^2 \, | \ldots | \, A^n)$ square of order n.

(i) $\alpha \in A^k$ column of Athen
$\det \left(A^1 | \ldots | A^{k-1} | \, \alpha A^k \, | \, A^{k+1} \, | \ldots | \, A^n\right) = \alpha \det A.$

(iii) If A has two equal columns $\det A = 0$.

(iv) $\det I_n = 1$.

(v) If A has a zero column $\det A = 0$.

(vi) If A has two parallel columns $\det A = 0$.

(vii) if some columns are linearly dependent $\det A = 0$.

(same properties for rows)

Matrices: determinant (properties)

$A = (A^1 | A^2 | \ldots | A^n)$ square of order n.

(viii) Swapping columns produces change in sign of the determinant

(ix) Adding to a column a multiple of another one does not chadnge the determinant

(x) If A is diagonal or triangular the determinant is the product of diagonal elements:

$$\det A = a_{11}a_{22}\cdots a_{nn}.$$

(xi) $\det A = 0$ iff columns are linearly dependent

(xii) $\det(AB) = \det A \det B$.

(same properties for rows)

Lesson 1: Basic scientific computing tools

1. Vectors (arrays)
2. Matrices
3. Linear systems

Linear systems: a linear equation …

b is the constant.

- A linear equation has the form $a_1x_1 + a_2x_2 + \cdots + a_nx_n = b$

$a_1, a_2, \ldots$ are called coefficients

x_i values are called unknowns (variables)

- a solution in tuple whiche verifies equation

$$x_1 + 3x_2 - x_5 = 2$$

Some solution vectors

$$(1, 1, 27, 53, 2), \quad (2, 3, \pi, 3, 9), \quad (0, 3, -15\pi, 0, 7)$$

Linear systems: more linear equations, i.e linear systems

Consider $m \geq 1$ linear equations sharing same $n \geq 1$ unknowns $x_1, x_2, \ldots, x_n$:

$$a_{i1}x_1 + a_{i2}x_2 + \cdots + a_{in}x_n = b_i \quad (i = 1, 2, \ldots, m)$$

a_{ij} coefficient of x_j in equation i, b_i constant of equation i

- a linear system of m equations in n unknowns has the form

$$\Sigma : \begin{cases} a_{11}x_1 + & a_{12}x_2 + & \cdots + & a_{1n}x_n = & b_1 \\ a_{21}x_1 + & a_{22}x_2 + & \cdots + & a_{2n}x_n = & b_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{m1}x_1 + & a_{m2}x_2 + & \cdots + & a_{mn}x_n = & b_m \end{cases}$$

- a vector $(\overline{x}_1, \overline{x}_2, \ldots, \overline{x}_n)$ is called solution of $\boldsymbol{\Sigma}$ iff is a solution of all equations

Linear systems: matrix form

- Let observe that if we denote by $A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \dots & \dots & \dots & \dots \\ a_{i1} & a_{i2} & \dots & a_{in} \\ \dots & \dots & \dots & \dots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}$ $x = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$ $b = \begin{pmatrix} b_1 \\ \dots \\ b_i \\ \dots \\ b_m \end{pmatrix}$

it is $\boxed{Ax = b.}$

- please note that to solve the system means to find coefficients used to express b as a linear combination of columns of A

Linear systems: linear systems with a unique solution

- if A is square Σ is said to be square. Rectangular otherwise.
- if A is square the system is said to be
  - singular if $\det A = 0$
  - nonsingular if $\det A \neq 0$,
- Theorem (Cramer): if A is nonsingular, linear systems $Ax = b$ will have a unique solution.
- methods for computing solution should take in account the structure of A
- We show three methods: one for diagonal systems, one for triangular systems and one for "full" systems

Linear systems: DIAGONAL SYSTEMS

What linear systems are fast to solve?

DIAGONAL SYSTEMS

$$
\begin{aligned}
a_{11}x_1 &= b_1\\
a_{22}x_2 &= b_2\\
a_{33}x_3 &= b_3\\
a_{44}x_4 &= b_4
\end{aligned}
$$

$$
\begin{pmatrix} a_{11} & & & \\ & a_{22} & & \\ & & a_{33} & \\ & & & a_{44} \end{pmatrix}
\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}
=
\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}
$$

Immediate solution

$$
x_1 = \frac{b_1}{a_{11}} \qquad x_2 = \frac{b_2}{a_{22}} \qquad x_3 = \frac{b_3}{a_{33}} \qquad x_4 = \frac{b_4}{a_{44}}
$$

Linear systems: TRIANGULAR SYSTEMS

TRIANGULAR SYSTEMS

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + a_{14}x_4 &= b_1 \\ a_{22}x_2 + a_{23}x_3 + a_{24}x_4 &= b_2 \\ a_{33}x_3 + a_{34}x_4 &= b_3 \\ a_{44}x_4 &= b_4 \end{aligned}$$

$\Leftrightarrow$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ & a_{22} & a_{23} & a_{24} \\ & & a_{33} & a_{34} \\ & & & a_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

1) $$x_4 = \frac{b_4}{a_{44}}$$

2) $$x_3 = \frac{b_3 - a_{34}x_4}{a_{33}}$$

3) $$x_2 = \frac{b_2 - a_{23}x_3 - a_{24}x_4}{a_{22}}$$

4) $$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3 - a_{14}x_4}{a_{11}}$$

Linear systems: TRIANGULAR SYSTEMS

IN GENERAL → **Backward Substitution Algorithm (matlab code)**

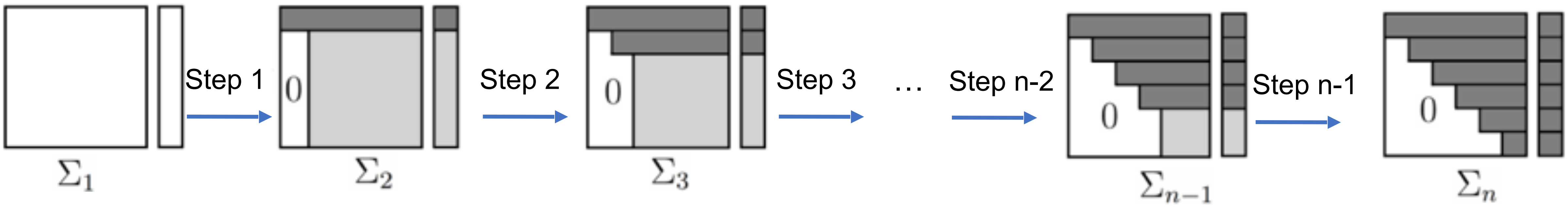
```
x(n)=b(n)/A(n,n)
for i=n-1:-1:1
     x(i)=b(i)
     for j=i+1:n
          x(i)=x(i)-A(i,j)*x(j)
     end
     x(i)=x(i)/A(i,i)
end
```

Linear systems: FULL SYSTEMS (Gaussian elimination)

Gaussian elimination method transforms a full system of n equations in a equivalent triangular one in n-1 steps

Idea

At step k, to subtract suitable vectors, multiple of equation k, to all equations at the bottom so that elements in column k under the diagonal element become 0



How to do this?

Linear systems: Gaussian Elimination

IN GENERAL → **Gaussian Elimination Algorithm (matlab code)**

```
for k=1:n-1
 for i=k+1:n
  M(i)= A(i,k)/A(k,k)
  for j=k+1:n
    A(i,j)=A(i,j)-M(i)*A(k,j)
  end
  b(i)=b(i)-M(i)*b(k)
 end
end
```

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Thanks for your attention

…… Digital Tech HPC continues