Vector and Matrix Notations

- $\mathbb{R}$: set of real numbers, also called **scalars** (0 order tensor)
  Examples: 1.5, 2, 0 . . .

  Vectorspace: defined over some field. Elements of field are called scalars.

- $\mathbb{R}^n$: space of vectors of length n (1st order tensor)
  Examples: $\begin{bmatrix} 0.5 \\ 2 \\ -1.3 \end{bmatrix} \in \mathbb{R}^3$

  $\mathbb{C}$

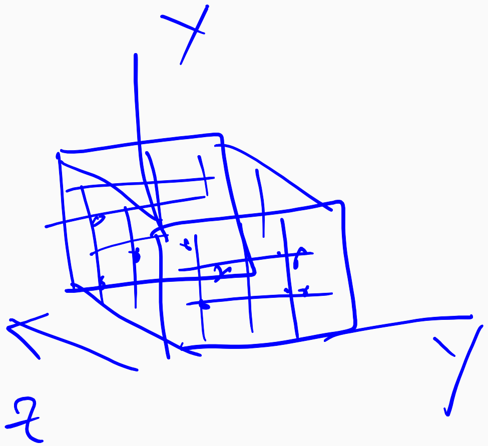
- What is a scalar in $\mathbb{C}^n$?

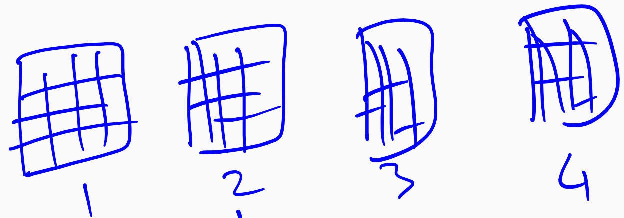
Vector and Matrix Notations

- $\mathbb{R}^{n\times n}$: matrix of dimensions $n \times n$ (2nd order tensor)
  Examples:

$$\begin{bmatrix} 1 & 0 & \pi \\ 3 & 2 & -0.2 \\ 1 & 3 & 2 \end{bmatrix} \in \mathbb{R}^{3\times 3}$$

- $\mathbb{R}^{n\times n\times n}$: 3D matrix of dimension $n \times n \times n$ (3rd order tensor)
  Examples:





z - slices

Later!

Basic vector operations:

1. Scalar times vector: $\alpha v, \quad v \in \mathbb{R}^n$

$\alpha \in \mathbb{R} \quad \alpha = 0.5, \quad v = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad \alpha v = \begin{bmatrix} 0.5 \\ 1 \\ 1.5 \end{bmatrix}$

2. Vector plus Vector: $u + v, \quad u, v \in \mathbb{R}^n$

$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} + \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} u_1 + v_1 \\ u_2 + v_2 \\ \vdots \\ u_n + v_n \end{bmatrix}$

3. Dot product: $u^T v, \quad u, v \in \mathbb{R}^n$

$\underbrace{[u_1, u_2, u_3, \dots u_n]}_{u} \underbrace{\begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}}_{v} = u_1 v_1 + u_2 v_2 + \dots + u_n v_n \in \mathbb{R}$

Basic Vector Operations:

1. Pointwise vector multiply: $u. * v$

   Example:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} .* \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} u_1 v_1 \\ u_2 v_2 \\ \vdots \\ u_n v_n \end{bmatrix}$$

2. Pointwise vector divide: $u./v$

   Example:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} ./ \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = \begin{bmatrix} u_1/v_1 \\ u_2/v_2 \\ \vdots \\ u_n/v_n \end{bmatrix}$$

$v_i \neq 0 \quad \forall i$

Basic Matrix Operations:

1. Matrix Transpose: A^T

   Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \qquad A^T = \begin{bmatrix} a_{11} & \cdots & a_{n1} \\ a_{12} & & a_{n2} \\ \vdots & & \vdots \\ a_{1n} & & a_{nn} \end{bmatrix}$$

2. Scalar times matrix: $\alpha A, \quad A \in \mathbb{R}^{n \times n}, \alpha \in \mathbb{R}$

   Example:

$$\alpha \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} \alpha a_{11} & \alpha a_{12} & \cdots & \alpha a_{1n} \\ \vdots & & & \vdots \\ \alpha a_{n1} & \alpha a_{n2} & \cdots & \alpha a_{nn} \end{bmatrix}$$

Basic Matrix Operations:

1. Matrix-Matrix addition: $A + B, \quad A, B \in \mathbb{R}^{m \times n}$

   Example:

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1n} \\ \vdots & & & \vdots \\ b_{n1} & b_{n2} & \cdots & b_{nn} \end{bmatrix} = \begin{bmatrix} a_{11}+b_{11} & a_{12}+b_{12} & \cdots & a_{1n}+b_{1n} \\ \vdots & & & \\ a_{n1}+b_{n1} & a_{n2}+b_{n2} & \cdots & a_{nn}+b_{nn} \end{bmatrix}$$

2. Matrix-vector multiplication: $Ax, \quad A \in \mathbb{R}^{n}, x \in \mathbb{R}^{n}$

   Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n \end{bmatrix}$$

Matrix vector multiplication: Row wise and Column wise

1. Row intepretation

$$\begin{bmatrix} — a_1^T — \\ — a_2^T — \\ \vdots \\ — a_n^T — \end{bmatrix} \begin{bmatrix} x \end{bmatrix} = \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_n^T x \end{bmatrix},$$

a_i^T : i^{th} row of A.

2. Column interpretation

$$\begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = x_1 a_1 + x_2 a_2 + \cdots + x_n a_n$$

a_i : i^{th} col of A

Note: if $x \neq 0$, but $Ax = 0$, then $\text{rank}(A) < n$

why?

BLAS-1,2,3

BLAS: Basic Linear Algebra Subroutines

1. Level-1 BLAS: saxpy operation:

Example

$$y \leftarrow y + \alpha x, \quad x, y \in \mathbb{R}^n, \ \alpha \in \mathbb{R}$$

$y = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \quad \alpha = 1.5, \quad x = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

$y = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + 1.5 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 2.5 \end{bmatrix}$

BLAS-1,2,3

BLAS: Basic Linear Algebra Subroutines

1. Level-2 BLAS:

$$y \leftarrow \alpha Ax + \beta y, \quad \alpha \in \mathbb{R},\ x, y \in \mathbb{R}^n,\ A \in \mathbb{R}^{n \times n}$$

Let $\alpha = 0.5$, $\beta = 0.1$

$A = \begin{bmatrix} 1 & 0 & 2 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}$, $x = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$, $y = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

$y = \alpha Ax + \beta y = 0.5 \begin{bmatrix} 1 & 0 & 2 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} + 0.1 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

$= 0.5 \begin{bmatrix} 3 \\ 1 \\ 1 \end{bmatrix} + 0.1 \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 0.5 \\ 0.5 \end{bmatrix} + \begin{bmatrix} 0 \\ 0.1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 1.5 \\ 0.5 \end{bmatrix}$

BLAS Level-3: Gaxpy operation:

$$C \leftarrow \alpha AB + \beta C, \quad \alpha \in \mathbb{R},\ A \in \mathbb{R}^{m\times n}, B \in \mathbb{R}^{n\times p},\ C \in \mathbb{R}^{m\times p}$$

Example: Let $\alpha = 1.0$, $\beta = 0.5$

$$A = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 0 \end{bmatrix}, \quad C = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 4 \\ 0 & 0 & 2 \end{bmatrix}$$

$$AB = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{bmatrix} \Rightarrow C = 1.0 \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & 2 \\ 1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 1 & 4 \\ 1 & 1 & 2 \end{bmatrix}$$

How to estimate cost of numerical algorithms?

FLOPS: Floating point operations:

A flop is a floating point add, subtract, multiply, or divide

Examples: $v, u \in \mathbb{R}^n$

$v + u$ Flops $= n$

$v .* u$ Flops $= n$

$AB = 2n^3$

$u^T v = 2n$ Flops

$Au = 2n^2$ Flops

$A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times n}$

Caution: FLOPS: Floating point ops per second

Used to select supercomputers: top500.org

ISC & SC conferences

Saxpy Operation: $y \leftarrow y + ax$

for $i = 1 : n$ **do**   1 Flop

$\quad y(i) = y(i) + ax(i)$ $\}$ 2 Flop $\Big\}$ 2n Flops

end for   1 Flop

Cost: $2n$

Rk: To calculate flops, find flops for innermost loop

Algorithm for dot product

$c = 0$

for $i = 1 : n$ **do**

$\quad c = c + x(i)y(i)$ 1 Flop 1 Flop 2 Flops 2n Flops

end for

Cost: 2n

Outer Product

Outer Product Operation: $u = xy^T$

Example:

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} y_1 & y_2, & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1y_1 & x_1y_2 & \cdots & x_1y_n \\ x_2y_1 & x_2y_2 & \cdots & x_2y_n \\ \vdots & & & \\ x_ny_1 & x_ny_2 & \cdots & x_ny_n \end{bmatrix}$$

It is a rank-1 matrix

Q why?

Ans: Each column can be obtained from a single column by a scalar multiplication

Outer Product Update

Outer Product Operation: $A = A + xy^T$

Example: $A \in \mathbb{R}^{3 \times 2}$

$x \in \mathbb{R}^4$, $y \in \mathbb{R}^3$

$\Rightarrow xy^T \in \mathbb{R}^{4 \times 3}$

Here, we can't add $A + xy^T$!

Gaxpy Operation: $y = y + Ax$ with Row-Oriented

for $i = 1 : m$ **do**
    for $j = 1 : n$ **do**
        $y(i) = y(i) + A(i, j)x(j)$ ← 2 Flops
        // Can you vectorize this inner loop?
    end for
end for

1 Flop   1 Flop

2n   2mn

Cost: 2mn

Dot Product Formulation: Which loop to vectorize for dot product formulation?

Colon Notation

$A(k,:)$ = k^{th} row of A

Let $A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix}$ $\quad A(2,:) = \begin{bmatrix} 5 & 6 & 7 & 8 \end{bmatrix}$

Note: These are Matlab Notations

$A(:,k)$ = k^{th} column of A

For above A:

$A(:,3) = \begin{bmatrix} 3 \\ 7 \\ 11 \end{bmatrix}$, $\quad A(2:3, 1:2) = \begin{bmatrix} 5 & 6 \\ 9 & 10 \end{bmatrix}$,

$A([1,3], 2:3) = \begin{bmatrix} 2 & 3 \\ 10 & 11 \end{bmatrix}$

Matrix Multiplication

ijk-version

for $i = 1 : m$ **do**
  for $j = 1 : n$ **do**
    for $k = 1 : p$ **do**
      $C(i,j) = C(i,j) + A(i,k)B(k,j)$ ← 2Flops } 2p } 2pn } 2pnm
    end for
  end for
end for

1 Flop

1 Flop

Cost: 2pmn

Other Variants:

Dot Product Formulation : Vectorize k loop :

for $i = 1:m$ do
  for $j = 1:n$ do
    $c(i,j) = c(i,j) + \underbrace{A(i, 1:p)}_{\text{row vector}} \underbrace{B(1:p, j)}_{\text{col vector}}$
  end for
end for

hence it is a dot product

Saxpy Formulation : Vectorize ith loop

for $j = 1 : n$
  for $k = 1 : p$
    $C(1:m, j) = \underbrace{C(1:m,j)}_{\text{col vector}} + \underbrace{A(1:m,k)}_{\text{col vector}}\underbrace{B(k,j)}_{\text{scalar}}$
  end
end

$\Rightarrow$ It is a saxpy operation!

Outer Product Formulation

Vectorize i & j loop

for k = 1 : p

$$c(i,j) = c(i,j) + \underbrace{A(1:m,k)}_{\text{column vector}}\,\underbrace{B(k,1:n)}_{\text{row vector}}$$

outer product

end

FLOPS: Floating Point Operations Per Second

1 FLOP = + or - or * or /

Operation	Dimension	Flops
$\alpha = x^T y$	$x, y \in \mathbb{R}^n$	
$y = y + ax$	$a \in \mathbb{R}, x, y \in \mathbb{R}^n$	
$y = y + Ax$	$A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^n, y \in \mathbb{R}^m$	
$A = A + yx^T$	$A \in \mathbb{R}^{m \times n}, x \in \mathbb{R}^n, y \in \mathbb{R}^m$	
$C = C + AB$	$A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{r \times n}, C \in \mathbb{R}^{m \times n}$	