MATRIX OPERATIONS

Numerical Linear Algebra (NLA)

Study of the approximate solution of fundamental problems from linear algebra by numerical methods that can be implemented on a computer

Basic problems in NLA

- Systems of Linear Equations
- Eigenvalue Problems

One of the most fundamental problems in NLA is to solve a system of m linear equations

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

for the n unknowns x_1, x_2, x_n. Often, but not necessarily, both coefficients and unknowns are real or complex numbers.

Many data fitting problems such as polynomial interpolation or least-squares fitting involve such a problem. Discretization of partial differential equations often yield also systems of linear equations that must be solved.

Systems of nonlinear equations are typically solved using iterative methods that solve a system of linear equations during each iteration.

Another basic problem in NLA is the eigenvalue problem which, given a matrix $\mathbf{A}$, consists of finding a non-zero vector $\mathbf{x}$ and a number λ such that

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

Coefficients of matrix $\mathbf{A}$, components of vector x and the number λ are often, but not necessarily, real or complex numbers.

Many applications in engineering, physics or chemistry such as geometrical transformations, quantum mechanics, vibrational analysis, or principal component analysis require the solution of an eigenvalue problem.

In this course we will use the following default notation:

- Boldface uppercase letters for matrices $\mathbf{A}$
- Boldface lowercase letters for vectors $\mathbf{x}$
- Italics lowercase latin or greek letters for numbers (scalars) x, λ

Due to lack of time we will limit our discussion to the case of matrices with real entries

ELEMENTARY LINEAR ALGEBRA

A vector space over a field F is a set V, with two operations + and $\cdot$ called vector addition and scalar multiplication, such that:

V is an abelian (commutative) group under +, that is:

$\mathbf{w} = \mathbf{u} + \mathbf{v}$ with $\mathbf{w} \in V$ for $\forall \mathbf{u}, \mathbf{v} \in V$	closure for +
$\mathbf{u} + (\mathbf{v} + \mathbf{w}) = (\mathbf{u} + \mathbf{v}) + \mathbf{w}$ for $\forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in V$	+ is associative
$\mathbf{u} + \mathbf{v} = \mathbf{v} + \mathbf{u}$ for $\forall \mathbf{u}, \mathbf{v} \in V$	+ is commutative
$\mathbf{0} + \mathbf{v} = \mathbf{v} + \mathbf{0} = \mathbf{v}$ for $\forall \mathbf{v} \in V$	neutral element for +
$\mathbf{v} + \overline{\mathbf{v}} = \overline{\mathbf{v}} + \mathbf{v} = \mathbf{0}$ with $\overline{\mathbf{v}} \in V$ for $\forall \mathbf{v} \in V$	inverse element for +

For any k in F and $\mathbf{v}$ in V the scalar product $k{\cdot}\mathbf{v}$ is an element of V subject to the following conditions:

$k\cdot(\mathbf{u}+\mathbf{v})=k\cdot\mathbf{u}+k\cdot\mathbf{v}$ for $\forall\,\mathbf{u},\mathbf{v}\in V$ and $\forall\,k\in F$ — distributivity for +

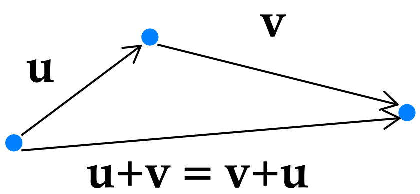
$(k+l)\cdot\mathbf{u}=k\cdot\mathbf{u}+l\cdot u$ for $\forall\,\mathbf{u}\in V$ and $\forall\,k,l\in F$ — distributivity for ·

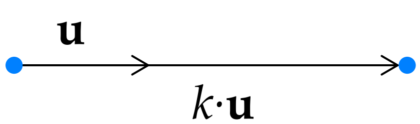
$k(l\cdot\mathbf{u})=(kl)\cdot\mathbf{u}$ for $\forall\,\mathbf{u}\in V$ and $\forall\,k,l\in F$ — associativity for ·

$1\cdot\mathbf{u}=\mathbf{u}$ for $\forall\,\mathbf{u}\in V$ — neutral element for ·

The elements of V are called vectors and those of the field F are called scalars.

Translations with the sequential performance as addition





Set of polynomials with real coefficients

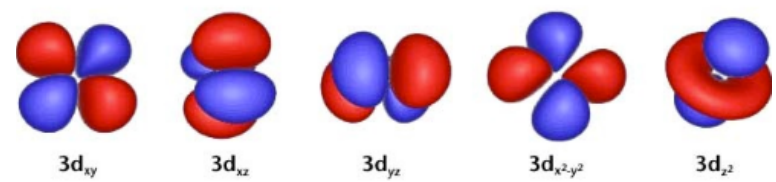
$$k(a_0 + a_1x + a_2x^2 + \ldots + a_nx^n) =$$
$$ka_0 + ka_1x + ka_2x^2 + \ldots + ka_nx^n$$

Set of n-tuples of real numbers R^n

$$\mathbf{u} = (a_1, a_2, a_3, \ldots, a_n)$$

$$(a_1, \ldots, a_n) + (b_1, \ldots, b_n) = (a_1+b_1, \ldots, a_n+b_n)$$
$$k(a_1, \ldots, a_n) = (ka_1, \ldots, ka_n)$$

Set of d-type hydrogenic orbitals



Since they are degenerate, any linear combination

$$\phi = c_1(xy)+c_2(xz)+c_3(yz)+c_4(x^2-y^2) +c_5(z^2)$$

is also a solution of the Schrödinger equation with the same energy

Definition

Let V be a vector space and $U \subseteq V$. If U is closed under addition and under scalar multiplication, we call U a subspace of V.

V and $\{\ \mathbf{0}\ \}$ are trivial subspaces of V

Definition

If $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ are in V and $k_1, k_2, \ldots, k_n$ are scalars, then the vector

$$k_1\mathbf{v_1} + k_2\mathbf{v_2} + \ldots + k_n\mathbf{v_n}$$

is called a linear combination of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$

The set of all linear combinations of $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ is a subspace of V, the subspace spanned by $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}$ or $sp(\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n})$

Definition

Let $S = \{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ be a set of distinct vectors in a vector space V. Then S is said to be linearly dependent if there are scalars $k_1, k_2, \ldots, k_n$, not all zero, such that

$$k_1\mathbf{v_1} + k_2\mathbf{v_2} + \ldots + k_n\mathbf{v_n} = \mathbf{0}$$

Obviously this is the same as saying that at least one of the vectors in S is a linear combination of the remaining ones.

The set S is said to be linearly independent iff

$$k_1\mathbf{v_1} + k_2\mathbf{v_2} + \ldots + k_n\mathbf{v_n} = \mathbf{0} \quad \text{implies} \quad k_1 = k_2 = \ldots = k_n = 0$$

This is the same as saying that no vector in S is equal to a linear combination of the other vectors in S.

Any set containing the vector $\mathbf{0}$ is linearly dependent, while the set $\{\ \mathbf{v}\ \}$ containing a single non-zero vector is linearly independent.

Definition

A linearly independent set of vectors $B = \{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ that span a vector space V is called a basis of V

Theorem

Any two bases of a vector space V have the same number of elements. If this number is finite we call V a finite-dimensional vector space of dimension n.

Lemma

If the set $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ spans V, it contains a basis of V

Lemma

If the set $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ is linearly independent, it can be expanded to a basis of V

Theorem

Let V have dimension n. Then,

- If $\{\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_n}\}$ is an independent set, it is already a basis of V.
- If $\{\mathbf{w_1}, \mathbf{w_2}, \ldots, \mathbf{w_n}\}$ spans V, it is a already a basis of V.

Definition

Let T and U be subspaces of V. The sum of T and U, denoted by $T+U$, is the set of all vectors $\mathbf{t}+\mathbf{u}$ where $\mathbf{t}$ is in T and $\mathbf{u}$ in U

Theorem

$T+U$ and $T \cap U$ are subspaces of V with

$$dim(T+U) = dim T + dim U - dim(T \cap U)$$

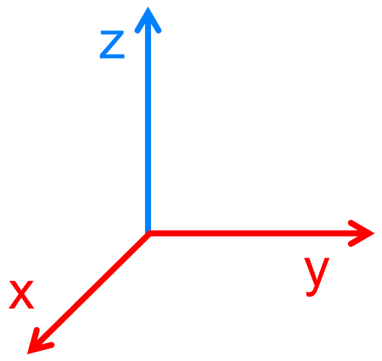
If $V = T + U$ and $T \cap U = \{\mathbf{0}\}$, then V is said to be the direct sum of T and U denoted by $T \oplus U$

Theorem

$V = T \oplus U$ iff every vector $\mathbf{v}$ in V can be written, in a unique manner, as a sum $\mathbf{v} = \mathbf{t} + \mathbf{u}$ where $\mathbf{t}$ is a vector in T and $\mathbf{u}$ one in U.

Example

Consider R^3 and $XY = sp\,\{ (1,0,0), (0,1,0) \}$ and $Z = sp\,\{ (0,0,1) \}$.



$R^3 = XY \oplus Z$

$dim(XY) = 2$

$dim(Z) = 1$

$dim(R^3) = dim(XZ) + dim(Z) = 3$

Definition

If U and V are vector spaces over a field F, a function $h : U \longrightarrow V$ is a homomorphism if it satisfies the following two conditions:

$$h(\mathbf{a}+\mathbf{b}) = h(\mathbf{a}) + h(\mathbf{b})$$
$$h(k \cdot \mathbf{a}) = k \cdot h(\mathbf{a})$$

A homomorphism between vector spaces is called a linear transformation or linear map.

If $h : U \longrightarrow V$ is a linear transformation

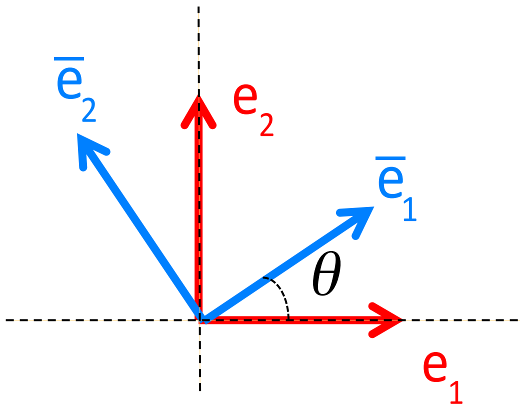
1. The kernel of U (all $\mathbf{a}$ in U such that $h(\mathbf{a}) = \mathbf{0}_V$) is a subspace of U called the null space of h
2. The range of h is a subspace of V

Definition

When $V = U$, the map $h : V \longrightarrow V$ is called a linear operator or an endomorphism of V.

Example

A (counterclockwise) rotation by an angle θ around a perpendicular axis passing through the origin is a linear operator in the Euclidean plane

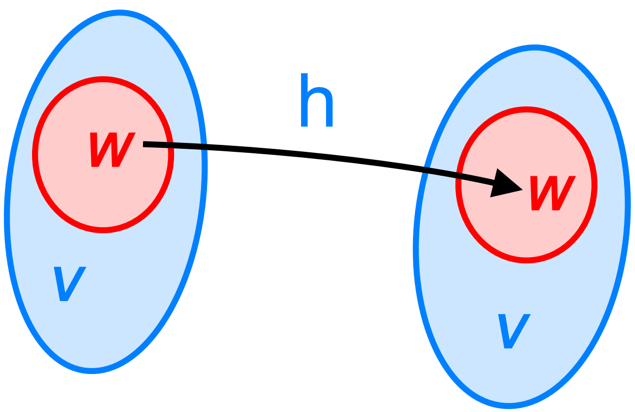


$$\bar{e}_1 = \cos\theta \cdot e_1 + \sin\theta \cdot e_2$$
$$\bar{e}_2 = -\sin\theta \cdot e_1 + \cos\theta \cdot e_2$$

Definition

A subspace W of a vector space V is said to be invariant under a linear map $h : V \longrightarrow V$ if h(W) is contained in W

In other words, any vector in an invariant subspace W of an endomorphism of V is sent to an image lying in the same subspace W.



Example

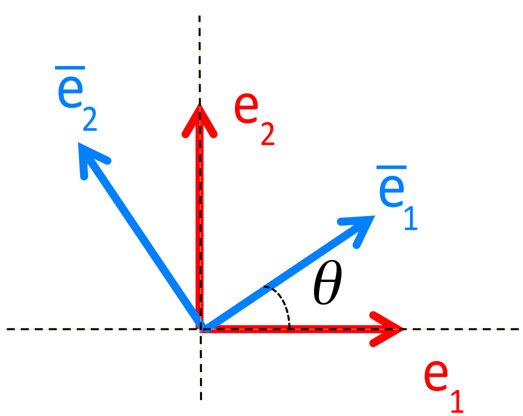
Consider a rotation around the z axis in $V = R^3$

Any vector (0,0,z) will be carried to (0,0,z) by the rotation while any vector (x,y,0) will be carried to a vector (x′,y′,0)

In this case, $W_1 = \{(0,0,z)\}$ and $W_2 = \{(x,y,0)\}$ are invariant subspaces of R^3 under the rotation

A linear transformation map $h: V \longrightarrow W$ where $\boldsymbol{dim(V)=n}$ and $dim(W)=m$ can be represented by a $n \times m$ matrix.

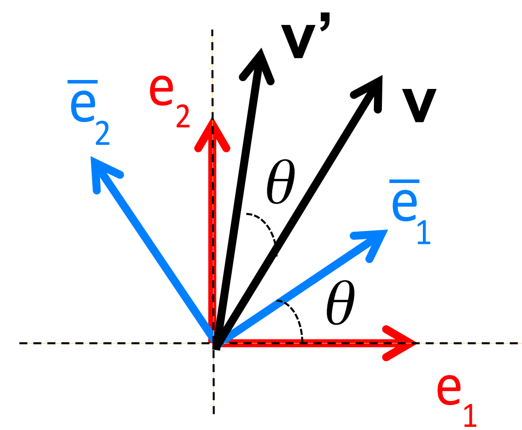
Effect of h on a basis



$$\bar{e}_1 = \cos\theta \cdot e_1 + \sin\theta \cdot e_2$$

$$\bar{e}_2 = -\sin\theta \cdot e_1 + \cos\theta \cdot e_2$$

Effect of h on the coordinates of a vector

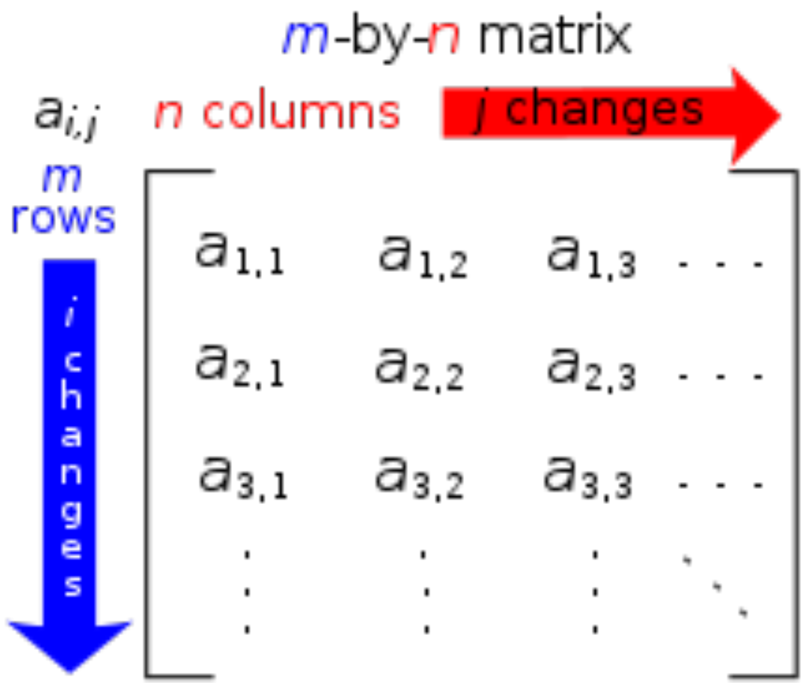


$$\mathbf{v} \longrightarrow \mathbf{v}' = \mathbf{R}\,\mathbf{v}$$

$$\begin{pmatrix} v'_1 \\ v'_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$

MATRIX MULTIPLICATION PROBLEMS

An $m \times n$ matrix is a rectangular array of numbers, symbols, or expressions arranged in m rows and n columns



The numbers, symbols, or expressions in the matrix are called its entries or elements. The size of the matrix is given by the number of rows m and columns n which are called the dimensions of the matrix.

The set of all $m \times n$ matrices R^{mxn} with real numbers as entries with the operations of matrix addition and multiplication of a matrix by a scalar form a vector space

Matrix addition

$$\mathbf{C} = \mathbf{A} + \mathbf{B} \qquad \begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix} + \begin{pmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & \ddots & \vdots \\ b_{m1} & \cdots & b_{mn} \end{pmatrix} = \begin{pmatrix} a_{11}+b_{11} & \cdots & a_{1n}+b_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1}+b_{m1} & \cdots & a_{mn}+b_{mn} \end{pmatrix}$$

$$c_{ij} = a_{ij}+b_{ij}$$

Matrix multiplication by a scalar

$$\mathbf{C} = \lambda\mathbf{A} \qquad \lambda\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mn} \end{pmatrix} = \begin{pmatrix} \lambda a_{11} & \cdots & \lambda a_{1n} \\ \vdots & \ddots & \vdots \\ \lambda a_{m1} & \cdots & \lambda a_{mn} \end{pmatrix}$$

$$c_{ij} = \lambda a_{ij}$$

In the following I will introduce some short homework assignments that are due before the practical session in the intensive course in which you will have to write short subroutines in FORTRAN programing language to do some of the basic matrix operations explained during the course.

Please do them and deposit your worked assignments in the MOODLE platform before we start the practical sessions in the intensive course.

For each assignment, please include the corresponding FORTRAN subroutine (only source code) with comment lines indicating your name, the function of the variables you use and any important information you consider that is necessary to follow your code. Please check before submitting your assignments that your subroutines really work by testing them with some examples. Include all subroutines in a single file with a main program calling them.

The exercise is to write your OWN matrix manipulation programs from scratch, so DO NOT USE matrix operations already included in the FORTRAN language.

1a) Scalar multiplication of a matrix

Write a SMUL(m,n,la,A,C) subroutine that should return in C the m x n matrix resulting from multiplying matrix A by the scalar contained in la.

1b) Matrix addition

Write a MADD(m,n,A,B,C) subroutine that should return in C the m x n matrix resulting from adding matrix A and matrix B.

A matrix in $R^{n \times n}$ is formed by $n \times n$ entries arranged in n rows and n columns
Vectors in R^n can be represented by either column matrices in $R^{n \times 1}$ or row matrices in $R^{1 \times n}$:

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

$$\mathbf{y} = \begin{pmatrix} y_1 & y_2 & y_3 \end{pmatrix}$$

In this course we will choose the column matrix representation for vectors in R^n.

In linear algebra, the transpose of a matrix $\mathbf{A}$ is an operator which flips a matrix over its diagonal, that is it switches the row and column indices of the matrix by producing another matrix denoted as $\mathbf{A}^{\mathrm{T}}$

$$\mathbf{A} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix} \longrightarrow \mathbf{A}^{T} = \begin{pmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{pmatrix}$$

Entries in $\mathbf{A}^{\mathrm{T}}$ and $\mathbf{A}$ are related by

$$(a_{ij})^{\mathrm{T}} = a_{ji}$$

The following relations hold for transposition:

$$(\mathbf{A}^{\mathrm{T}})^{\mathrm{T}} = \mathbf{A} \qquad (\mathbf{A}+\mathbf{B})^{\mathrm{T}} = \mathbf{A}^{\mathrm{T}} + \mathbf{B}^{\mathrm{T}} \qquad (\lambda\mathbf{A})^{\mathrm{T}} = \lambda\mathbf{A}^{\mathrm{T}}$$

Matrices with the same number n of rows and columns are called square matrices.

Special square matrices:

$$\mathbf{D} = \begin{pmatrix} d_{11} & 0 & 0 \\ 0 & d_{22} & 0 \\ 0 & 0 & d_{33} \end{pmatrix} \qquad \mathbf{U} = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} u_{11} & 0 & 0 \\ u_{21} & u_{22} & 0 \\ u_{31} & u_{32} & u_{33} \end{pmatrix}$$

Diagonal | Upper triangular | Lower triangular

$$\mathbf{S} = \begin{pmatrix} 3 & 1 & 5 \\ 1 & 2 & 0 \\ 5 & 0 & 5 \end{pmatrix} \qquad \mathbf{K} = \begin{pmatrix} 0 & 1 & 5 \\ -1 & 0 & -2 \\ -5 & 2 & 0 \end{pmatrix}$$

Symmetric: $\mathbf{S}^{\mathrm{T}} = \mathbf{S}$

Skew-symmetric $\mathbf{K}^{\mathrm{T}} = -\mathbf{K}$

For a square matrix $\mathbf{A}$, the sum of its entries in the diagonal is called the trace of the matrix

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \longrightarrow \quad Tr(\mathbf{A}) = a_{11} + a_{22} + a_{33}$$

In general, for the $n \times n$ case:

$$Tr(\mathbf{A}) = \sum_{i=1}^{n} a_{ii}$$

2a) Transpose of a matrix

Write a TRANS(m,n,A,AT) subroutine that should return in AT the n x m matrix resulting from transposing the m x n matrix

2b) Symmetric matrix

Write a SYM(n,S,f) subroutine that should return 1 in f if S is a symmetric n x n matrix, -1 if it is skew-symmetric, and 0 otherwise.

2c) Trace of a matrix

Write a TRA(n,A,t) subroutine that should return the trace of the n x n matrix A in variable t.

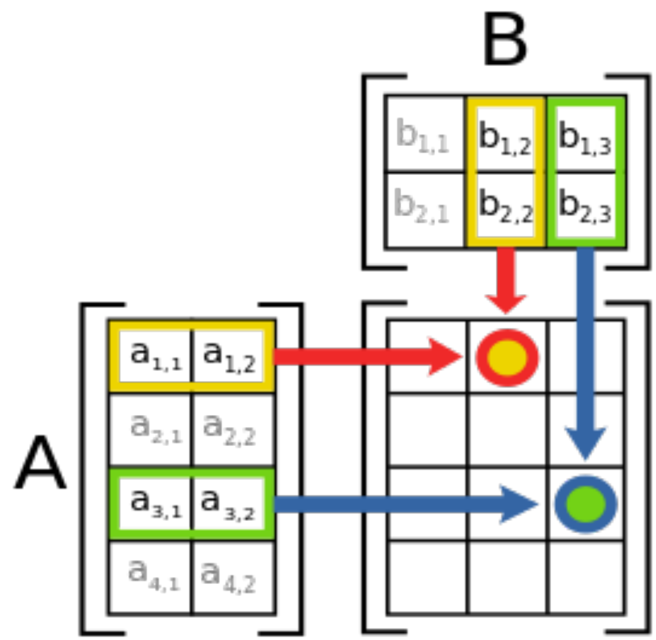
We define the product of a $m \times n$ matrix $\mathbf{A}$ times a $n \times p$ matrix $\mathbf{B}$ as the $m \times p$ matrix $\mathbf{C} = \mathbf{AB}$ whose entries are

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

Practical example:

$$\overset{4\times 2 \text{ matrix}}{\begin{bmatrix} a_{11} & a_{12} \\ \cdot & \cdot \\ a_{31} & a_{32} \\ \cdot & \cdot \end{bmatrix}} \overset{2\times 3 \text{ matrix}}{\begin{bmatrix} \cdot & b_{12} & b_{13} \\ \cdot & b_{22} & b_{23} \end{bmatrix}} = \overset{4\times 3 \text{ matrix}}{\begin{bmatrix} \cdot & x_{12} & x_{13} \\ \cdot & \cdot & \cdot \\ \cdot & x_{32} & x_{33} \\ \cdot & \cdot & \cdot \end{bmatrix}}$$

$$x_{12} = a_{11} b_{12} + a_{12} b_{22}$$
$$x_{33} = a_{31} b_{13} + a_{32} b_{23}$$



2a) Matrix product update

Write a GEMM(m,n,p,al,A,B,be,C) subroutine that should return in C the update of the m x p matrix C given by

$$C = \alpha \mathbf{A}\mathbf{B} + \beta \mathbf{C}$$

where A is a m x n matrix, B a n x p matrix and al, be two real scalars

Some properties of matrix multiplication

For general matrices

$$\mathbf{AB} \neq \mathbf{BA}$$

non commutative

$$\mathbf{A}(\mathbf{B}+\mathbf{C}) = \mathbf{AB}+\mathbf{AC}$$

$$(\mathbf{A}+\mathbf{B})\mathbf{C} = \mathbf{AC}+\mathbf{AC}$$

distributive over matrix addition

$$\lambda(\mathbf{AB}) = (\lambda\mathbf{A})\mathbf{B} = \mathbf{A}(\lambda\mathbf{B})$$

compatible with scalar multiplication

$$(\mathbf{AB})^T = \mathbf{B}^T\mathbf{A}^T$$

Trace of a product

Identity matrix

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} \longrightarrow \mathbf{AI} = \mathbf{IA}$$

Inverse matrix

$$\mathbf{AA}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

If A^{-1} exists then A is said to be invertible, if not, then A is said to be singular.

Assuming $a \in R$ and $\mathbf{x}, \mathbf{y}, \mathbf{z} \in R^n$ the fundamental vector operations are:

Scalar multiplication	$\mathbf{z} = a\mathbf{x}$	$\Rightarrow$	$z_i = a x_i$
Vector addition	$\mathbf{z} = \mathbf{x} + \mathbf{y}$	$\Rightarrow$	$z_i = x_i + y_i$
Dot product	$a = \mathbf{x}^{\mathrm{T}} \mathbf{y}$	$\Rightarrow$	$a = \sum_{i=1}^{n} x_i y_i$
Hadamard product	$\mathbf{z} = \mathbf{x} * \mathbf{y}$	$\Rightarrow$	$z_i = x_i y_i$
axpy update	$\mathbf{y} = a\mathbf{x} + \mathbf{y}$	$\Rightarrow$	$y_i = a x_i + y_i$

4a) Scalar vector multiplication

Write a SCAL(n,a,x,y) subroutine that should return in y the result of multiplying vector x of dimension n by the scalar in a.

4b) Dot product

Write a DOT (n,d,x,y) subroutine that should return the dot product of n-dimensional vectors x and y in variable d.

4c) Axpy update

Write a AXPY(n,a,x,y) subroutine that should return the axpy update of vector y.

We have seen that the dot product of two vectors yielding a scalar value can be written as a matrix product of a row matrix times a column matrix:

$$a = \mathbf{x}^{\mathrm{T}}\mathbf{y} \qquad \Rightarrow \qquad a = \sum_{i=1}^{n} x_i y_i$$

If we multiply the vectors in the column-row order, the result is a matrix:

$$\mathbf{A} = \mathbf{x}\mathbf{y}^{\mathrm{T}} \qquad \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \begin{pmatrix} 4 & 5 \end{pmatrix} = \begin{pmatrix} 4 & 5 \\ 8 & 10 \\ 12 & 15 \end{pmatrix}$$

This operation is called the outer product of the two vectors.

The fundamental matrix-vector operations are:

Generalized *axpy* update (*gaxpy*):

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{y} \qquad \Rightarrow \qquad y_i = \sum_{j=1}^{n} ax_{ij} + y_i$$

Outer product update:

$$\mathbf{A} = \mathbf{A} + \mathbf{x}\mathbf{y}^T$$

5a) Gaxpy update

Write a GAXPY(m,n,A,x,y) subroutine to perform a Gaxpy update of m-dimensional vector y using the m x n matrix a and the n-dimensional vector x.

5b) Outer product update

Write a OUTP (m,x,n,y,A) subroutine that should update the $m \times n$ matrix A using the outer product of m-dimensional vector x and n-dimensional vector y.

MATRIX DETERMINANTS

The determinant of an $n \times n$ matrix $\mathbf{A}$, denoted by $\det(\mathbf{A})$ or $|\mathbf{A}|$ is defined as follows:

If $n = 1$

$$\det(\mathbf{A}) = a_{11}$$

If $n > 1$

$$\det(\mathbf{A}) = \sum_{j=1}^{n} a_{ij}(-1)^{i+j}\det(M_{ij}) \quad 1 \leq i \leq n$$

where $\mathbf{M}_{\mathrm{ij}}$, called a minor of $\mathbf{A}$, is the matrix obtained by removing row i and column j of $\mathbf{A}$

The determinant of a 2×2 matrix is:

$$|A| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc.$$

and for a 3×3 matrix:

$$|A| = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a \begin{vmatrix} e & f \\ h & i \end{vmatrix} - b \begin{vmatrix} d & f \\ g & i \end{vmatrix} + c \begin{vmatrix} d & e \\ g & h \end{vmatrix}$$
$$= aei + bfg + cdh - ceg - bdi - afh$$

From a computational viewpoint this way of calculating higher order determinants is not practical since it leads to a recursive algorithm that needs $O(n!)$ floating point operations.

6) Calculation of determinants for nxn matrices with $n \leq 3$

Write a DET(n,A,d) subroutine to calculate the determinant d of matrix A where $n \leq 3$ is the dimension of the matrix.

The following relations between the determinants of related matrices are interesting for the development of efficient algorithms to calculate determinants of matrices

- If any row or column of $\mathbf{A}$ has only zero entries, then $det(\mathbf{A}) = 0$
- If any two rows or columns of $\mathbf{A}$ are the same, then $det(\mathbf{A}) = 0$
- If $\mathbf{A'}$ is obtained from $\mathbf{A}$ by adding a multiple of a row(column) of $\mathbf{A}$ to another row (column), then $det(\mathbf{A'}) = det(\mathbf{A})$
- If $\mathbf{A'}$ is obtained from $\mathbf{A}$ by interchanging two rows (columns) of $\mathbf{A}$, then $det(\mathbf{A'}) = -\, det(\mathbf{A})$
- If $\mathbf{A'}$ is obtained from $\mathbf{A}$ by scaling a row (column) of $\mathbf{A}$ by λ then $det(\mathbf{A'}) = \lambda\, det(\mathbf{A})$

The following properties of determinants are important in order to develop efficient algorithms to calculate the determinant of a matrix

- If $\mathbf{A}$ and $\mathbf{B}$ are two $n \times n$ matrices, then $det(\mathbf{AB}) = det(\mathbf{A})\, det(\mathbf{B})$
- $det(\mathbf{A}^{\mathrm{T}}) = det(\mathbf{A})$
- If $\mathbf{A}$ is non-singular, then $det(\mathbf{A}^{-1}) = (det(\mathbf{A}))^{-1}$
- If $\mathbf{A}$ is a triangular $n \times n$ matrix (either lower or upper) then

$$\det(\mathbf{A}) = \prod_{i=1}^{n} a_{ii}$$

$$U = \begin{bmatrix} 1 & -1 & 0 & 5 \\ 0 & 2 & 3 & -6 \\ 0 & 0 & -4 & 7 \\ 0 & 0 & 0 & 8 \end{bmatrix} \longrightarrow \det(U) = 1(2)(-4)(8) = -64.$$

The best-known application of the determinant is the fact that it indicates whether a matrix $\mathbf{A}$ is nonsingular, or invertible. The following statements are all equivalent:

If $det(\mathbf{A}) \neq 0$

- $\mathbf{A}$ is nonsingular
- $\mathbf{A}^{-1}$ exists
- The system $\mathbf{Ax} = \mathbf{b}$ has a unique solution for any n-vector $\mathbf{b}$
- The system $\mathbf{Ax} = \mathbf{0}$ has only the trivial solution $\mathbf{x} = \mathbf{0}$

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