Vectors

Kindergarten: vector = $(v_1,\dots,v_n)$, $v_i\in\mathbb{R}$
Quantum kindergarten: $v_i\in\mathbb{C}$

Mathematics: **vector space** (linear space) is defined by the axioms:

For vectors u, v, w and numbers $a, b \in \mathbb{R}$ or $\mathbb{C}$ (a field[a] in general):

$$\left.\begin{array}{rcl} u+(v+w) &=& (u+v)+w \\ u+v &=& v+u \\ \exists \text{ null vector } 0: v+0 &=& v \\ \exists \text{ opposite vector } -v: v+(-v) &=& 0 \\ a(bv) &=& (ab)v \\ 1v &=& v \\ a(u+v) &=& au+av \\ (a+b)v &=& av+bv \end{array}\right\}\text{as in } \mathbb{R}$$

Notation: v, $\mathbf{v}$, $\vec{v}$ (real in 2D, 3D), $\underline{v}$, $|v\rangle$ ("ket"), v_i (?)

[a]česky komutativní těleso

Linear dependence

A set of nonzero vectors $v^{(i)}$, $i=1..m$, is **linearly dependent** if there is a null linear combination with at least one of a_i nonzero:

$$\sum a_i v^{(i)} = 0$$

A linearly independent set of vectors such that any vector (of given space) can be expressed as its linear combination is called a **basis**

$$v = \sum v_i b^{(i)}$$

Example. Are the following vectors in $\mathbb{R}^4$ linearly dependent? see mmpc1.mw

$$(1,2,3,4)^\top, (1,-2,3,-4)^\top, (1,0,1,0)^\top$$

no

Example. Are the following vectors in $\mathbb{C}^2$ linearly dependent?

$$\begin{pmatrix} i \\ 1 \end{pmatrix}, \begin{pmatrix} 1+i \\ 1-i \end{pmatrix}$$

yes

Example. Consider a linear space of functions of $x\in[0,2\pi]$ with basis $\{1,\cos(x),\cos(2x),\cos(3x),\dots\}$. Can function $\cos^2(x)$ be expressed in this basis?

yes: $\{1/2, 0, 1/2, 0, 0, \dots\}$

Scalar (inner, dot) product

We need a richer structure!

Kindergarten: scalar product $\vec{u}\cdot\vec{v} = \sum u_i v_i$

Mathematics: (u,v) is a number (real, complex) obeying axioms:

$$\begin{array}{rcl} (u,v) &=& (v,u)^* \ (^* = \text{complex conjugate}) \\ (au,v) &=& a^*(u,v) \quad \text{(in physics)} \quad \Rightarrow \quad (u,av) = a(u,v) \\ &=& a(u,v) \quad \text{(in mathematics)} \Rightarrow \quad (u,av) = a^*(u,v) \\ (u+v,w) &=& (u,w)+(v,w) \\ (u,u) &\ge& 0 \\ (u,u)=0 &\Rightarrow& u=0 \text{ (null vector)} \end{array}$$

Notation: $u^\top v$, $u^\top\cdot v$, $u^\dagger v$,[b] (u,v), $\langle u,v\rangle$, $\vec{u}\cdot\vec{v}$, $\boldsymbol{u}\cdot\mathbf{v}$, $\langle u|v\rangle$ (bra-ket), $u_i v^i$ (covector-vector)
$\cdot$ (real spaces) or $|$ (complex spaces) = sum over a pair of indices

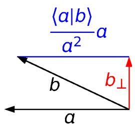
Definition: If $(u,v)=0$, vectors u, v are **perpendicular**

$(u,u)^{1/2} = |u| = \|u\|$ = norm[c]

[b]symbol † = transpose + complex conjugate = adjoint = Hermitean (Hermitian) conjugate
[c]similar space with a norm only (and complete) = Banach space; under some conditions $(u,v) = (|u+v|^2 - |u-v|^2)/4$

(Cauchy–)Schwarz inequality

Dot-product in $\mathbb{R}^n$: $\vec{x}\cdot\vec{y} = |\vec{x}||\vec{y}|\cos\theta \equiv xy\cos\theta \le xy$.
For nonzero a, b (zero cases are trivial):[d]



$$b_\perp = b - \frac{\langle a|b\rangle}{a^2}a \quad \Rightarrow \quad \langle a|b_\perp\rangle = \langle a|b - \frac{\langle a|b\rangle}{a^2}a\rangle = \langle a|b\rangle - \frac{\langle a|b\rangle}{a^2}\langle a|a\rangle = 0$$

$$b = \frac{\langle a|b\rangle}{a^2}a + b_\perp$$

Pythagoras[e]:

$$b^2 = \left(\frac{|\langle a|b\rangle|}{a^2}\right)^2 a^2 + b_\perp^2 \ge \left(\frac{|\langle a|b\rangle|}{a^2}\right)^2 a^2 = \frac{|\langle a|b\rangle|^2}{a^2}$$

$$a^2b^2 \ge |\langle a|b\rangle|^2 \quad \Rightarrow \quad \boxed{|a||b| \ge |\langle a|b\rangle|} \overset{\mathbb{R}}{\ge} \langle a|b\rangle$$

| | has two meanings: |complex number| and |vector|

$\Rightarrow$ **triangle inequality** (in $\mathbb{R}$)

$$|a+b| \le |a|+|b| \quad \text{or} \quad |x-z| \le |x-y| + |y-z|$$

i.e., $|a-b|$ is a **metric**.

[d]Common shortcut: $a^2 \equiv |a|^2 = \langle a|a\rangle$
[e]In complex spaces: $\langle b|a\rangle^* = \langle a|b\rangle$ and for scalar $c\in\mathbb{C}$ it holds $|ca|^2 = \langle ca|ca\rangle = c^*c\langle a|a\rangle = |c|^2|a|^2$

Hilbert space

Hilbert space = linear space with a scalar product which is:

example of not-complete space: finite linear combinations of $\{(1,0,0,\dots),(0,1,0,\dots),(0,0,1,\dots),\dots\}$

- complete (any Cauchy sequence[f] converges in the (u,u) metric)
- usually also separable (it contains a countable dense subset $\Rightarrow$ there is a countable basis)

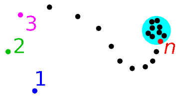
Loosely: "no vector is missing"
"it is not too big" or "there are no problems with using infinite sums"

Any finite vector space is a Hilbert space.

Example. Wavefunction is a vector of a Hilbert space, $\int|\psi(\boldsymbol{\tau})|^2\mathrm{d}\boldsymbol{\tau}$ must be finite[g]. The scalar product is:

$$\langle\phi|\psi\rangle = \int \phi(\boldsymbol{\tau})^*\,\psi(\boldsymbol{\tau})\mathrm{d}\boldsymbol{\tau}$$

n bosons: $\boldsymbol{\tau}\in\mathbb{R}^{3n}$, n fermions (chemistry): $\boldsymbol{\tau}\in(\mathbb{R}\times\{\alpha,\beta\})^{3n}$



[f]Sequence $\{v_i\}_{i=1}^\infty$ is Cauchy if $\forall d>0\ \exists n: |v_j - v_i| < d\ \forall i,j>n$. → → →
[g]For bound states , cf. de Broglie free-space "matter waves" . . .

Orthogonal and orthonormal bases

Orthogonal basis = all vectors are perpendicular.
Orthonormal basis = also normalized.

$$b^{(i)}\cdot b^{(j)} = \delta_{ij}$$

Components of v in an orthonormal basis:

$$v_i = v\cdot b^{(i)} \Rightarrow v = \sum v_i b^{(i)} = (v_1,\dots,v_n)_b$$

Scalar product:

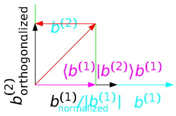
$$u\cdot v = \sum u_i v_i$$

Scalar product in $\mathbb{C}$ in physics

$$\langle u|v\rangle = \sum u_i^* v_i$$

Gram–Schmidt orthogonalization

A general basis $b^{(i)}$ can be orthogonalized by the Gram–Schmidt algorithm:



$$\begin{array}{rcl} b^{(1)} &:=& b^{(1)}/|b^{(1)}| \\ b^{(2)} &:=& b^{(2)} - \langle b^{(1)}|b^{(2)}\rangle b^{(1)},\ b^{(2)} := b^{(2)}/|b^{(2)}| \\ b^{(3)} &:=& b^{(3)} - \langle b^{(1)}|b^{(3)}\rangle b^{(1)} - \langle b^{(2)}|b^{(3)}\rangle b^{(2)},\ b^{(3)} := b^{(3)}/|b^{(3)}| \end{array}$$

":=" means "assign to" as in computer code.

Bases used in a Hilbert space are usually orthogonal or orthonormal

Example. Find all orthonormal bases $\{b^{(1)}, b^{(2)}\}$ in $\mathbb{C}^2$ for $b^{(1)} = (1,i)/\sqrt{2}$ ($b_1^{(1)} = 1$, $b_2^{(1)} = i$)

$$\left\langle\begin{pmatrix}1\\i\end{pmatrix}\middle|\begin{pmatrix}x\\y\end{pmatrix}\right\rangle = x - iy \overset{!}{=} 0 \quad\Rightarrow\quad x = iy \quad\Rightarrow\quad b^{(2)} = \frac{c}{\sqrt{2}}\left|\begin{pmatrix}i\\1\end{pmatrix}\right\rangle, |c| = 1$$

Remember complex conjugate in the dot product, $i^* = -i$

more examples: see mmpc1.mw

Another notation: $\left|\begin{matrix}1\\i\end{matrix}\right\rangle^\dagger = \left\langle\begin{matrix}1\\-i\end{matrix}\right|$

Linear forms

Linear form f (linear operator) assigns a number $f(v)\in\mathbb{R}$ (or $\mathbb{C}$) to a vector.

Axioms: for linear forms f, g, number a, and a vector v:

$$\begin{array}{rcl} (f+g)(v) &=& f(v)+g(v) \\ f(av) &=& af(v) \end{array}$$

For finite n one can write (In infinite-dimension spaces there may be continuity problems):

$$f(u) = \sum_{i=1}^n f_i u_i$$

Otherwise in Hilbert spaces linear form ≈ scalar product:

$$f(v) = \sum f_i v_i = (f^*, v)$$

Linear form in Euclidean spaces (in some context) = covector, dual vector, covariant vector ("normal" vector = contravariant vector)

- vector = column vector,
- covector = row vector (transposed) $f^\top$, inverse transformation if a basis changes

Scalar product then is: $f(u) = f^\top\cdot u = f^\top u = f^i u_i$ (Einstein summation convention).
In complex Hilbert spaces $^\top \to {}^\dagger$

Covector example

Example. Force $\vec{F}$ = covector, path $\mathrm{d}\vec{s}$ = vector.

$$\vec{F} = -\vec{\nabla}U, \quad \mathrm{d}W = \vec{F}\cdot\mathrm{d}\vec{s}$$

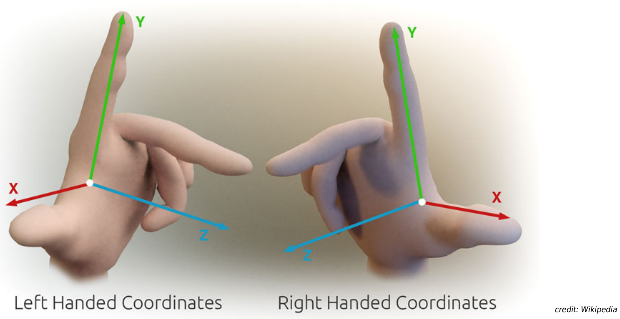
Units: $[\vec{F}]$ = energy/length, $[\mathrm{d}\vec{s}]$ = length.

If length unit changes from m to cm, $\mathrm{d}\vec{s}$ multiplies 100×, but (if the energy unit remains the same) $\vec{F}$ multiplies 0.01×.

Maple

In package LinearAlgebra, operator "." is used for scalar product:
`covector.vector`
`rows.columns` (in matrix multiplication)
`^+` = transposition
`^*` = Hermitean conjugate

3D: Right- and left-handed coordinate system



Right-handed: math, science, technology (Maple default)
Left-handed: 3D image processing (Micro$oft Direct 3D, PovRay)

Matrices

Square matrix $n \times n$, e.g.:

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

may represent:

- matrix of coefficients of a set of n of linear equations for n unknowns:
$$\sum_j A_{ij} x_j = b_i \quad \text{or} \quad A \cdot x = b \quad \text{or} \quad Ax = b \quad \text{or} \quad |\hat{A}|x\rangle = |b\rangle$$
- linear transformation (map, operator) $\mathbb{R}^n \to \mathbb{R}^n$ or $\mathbb{C}^n \to \mathbb{C}^n$
$$x_i \to \sum_j A_{ij} x_j \quad \text{or} \quad x \to A \cdot x \quad \text{or} \quad x \to Ax \quad \text{or} \quad |x\rangle \to |\hat{A}|x\rangle$$
- matrix of coefficients of a quadratic form $\mathbb{R}^n \to \mathbb{R}$ or $\mathbb{C}^n \to \mathbb{C}$
$$x_i \to \sum_{ij} x_i A_{ij} x_j \quad \text{or} \quad x \to x^\mathsf{T} \cdot A \cdot x \quad \text{or} \quad x \to x^\mathsf{T} A x \quad \text{or} \quad |x\rangle \to \langle x|\hat{A}|x\rangle$$
- a quadratic tensor; e.g., of pressure or small deformation

Unitary matrix

Orthogonal[h] (in $\mathbb{R}^n$) or **unitary** (in $\mathbb{C}^n$) matrix is a square matrix for which:

$$U^\mathsf{T} \cdot U = \delta \quad \text{or} \quad U^\dagger \cdot U = \delta$$

or in coordinates

$$\sum_j U^\mathsf{T}_{ij} U_{jk} = \sum_j U_{ji} U_{jk} = \delta_{ik} \quad \text{or} \quad \sum_j U^\dagger_{ij} U_{jk} = \sum_j U^*_{ji} U_{jk} = \delta_{ik}$$

- columns U_{*i} can be treated as coordinates of an orthonormal basis (in other orthonormal basis), i.e., a (matrix of) unitary transformation
- U is regular: $U^{-1} = U^\dagger$
- $|\det U| = 1$ (in $\mathbb{C}$); in $\mathbb{R}$ this means that $\det U = \pm 1$
- a unitary matrix transforms an orthonormal basis to an orthonormal basis
- linear map $x \to U \cdot x$ "preserves angles", in $\mathbb{R}$ it can be interpreted as:
  - rotation in $\mathbb{R}^n$ (for $\det U = 1$)
  - rotation and reflection in $\mathbb{R}^n$ (for $\det U = -1$).

Examples of linear transformations in $\mathbb{R}^n$ useful in molecular chemistry: `mmpc1.mw`

[h] term "orthonormal" is not used

Matrices

Notation:

- In quantum theory often denoted as $\hat{A}$
- Other habits (e.g., as tensors): $\overleftrightarrow{A}$, $\underline{A}$
- $A \cdot x$ is less common than Ax;
  in the bra-ket notation $A|x\rangle$ or $|Ax\rangle$ or $|A|x\rangle$
- Vectors u and co-vectors u^T or $u^\dagger \equiv \langle u|$ ("bra") should be distinguished.

Matrices in infinite-dimension spaces are infinite = linear operators

If the set of equations $A \cdot x = b$ can be solved $\forall b$, then A is called **regular**. The solution is then:

$$x = A^{-1} \cdot b$$

where A^{-1} = **inverse matrix**, $A \cdot A^{-1} = A^{-1} \cdot A = \delta$, and $\delta = \text{diag}(1, 1, \ldots)$ = **unit matrix**, identity matrix, in coordinates Kronecker delta, also written as E, $\mathbb{1}$, $\boldsymbol{I}$, I, $\overleftrightarrow{I}$, etc.

Examples. Invert matrices:

a) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}$, **b)** $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$

a) $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 0 \\ 0 & 0 & 1/3 \end{pmatrix}$, **b)** $\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}$

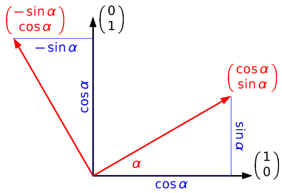
Matrix of rotation

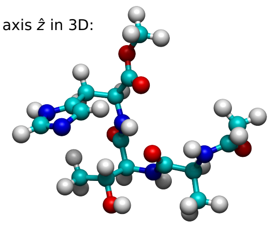
Matrix of rotation by oriented angle $+\alpha$ in 2D:

$$\begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}$$

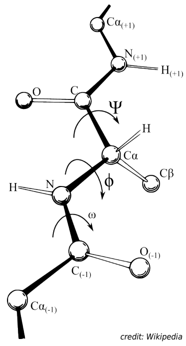
Matrix of rotation by angle α around axis $\hat{z}$ in 3D:

$$\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$





Internal coordinates:



Determinant

Determinant of a square matrix A is the number defined as a sum over all $n!$ permutations p of indices $\{1, 2, \ldots, n\}$:

$$\det A = \sum_p \text{sign}(p) \prod_i A_{i,p(i)}$$

where $\text{sign}(p) = (-1)^{\text{number of transpositions in } p}$.

$\det A \neq 0$ for a regular matrix.

It holds

$$\det(A \cdot B) = \det(A)\det(B), \quad \det(A^{-1}) = \frac{1}{\det A} \quad \text{(for regular } A)$$

The determinant of a diagonal or triangular matrix = product of the numbers on the diagonal

Example. Calculate a) $\text{sign}(2, 3, 1)$, b) $\text{sign}(n, n-1, n-2, \ldots, 2, 1)$

a) 1, b) $(-1)^{n(n-1)/2}$ (= 1 for $n \equiv 0, 1$ mod 4 and −1 otherwise)

Example

Write a matrix of rotation by angle α around vector $(a, b, c)^T$

- Use spherical coordinates:
  $(a, b, c) = (r \sin\theta \cos\varphi, r \sin\theta \sin\varphi, r \cos\theta)$
  reverse: $r = \sqrt{a^2 + b^2 + c^2}$, $\theta = \arccos(c/r)$, $\varphi = \arctan(b, a)$
  Overloaded function $\arctan(b, a) = \arctan(b/a) + k\pi$, where k is such integer that $\varphi = \arctan(b, a)$ is in the correct quadrant. In Fortran and C called `atan2`.
- Compose from right (= in the order it is applied to a vector):
  R_1^{-1} = rotation by $-\varphi$ around $\hat{z}$
  R_2^{-1} = rotation by $-\theta$ around $\hat{y}$
  R_3 = rotation by α around $\hat{z}$
  R_2 = rotation by θ around $\hat{y}$
  R_1 = rotation by φ around $\hat{z}$
- Rotation matrix

$$R = R_1 \cdot R_2 \cdot R_3 \cdot R_2^{-1} \cdot R_1^{-1}$$

see mmpc1.mw