Vectors

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

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

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

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 $\mathbb{R}^3$ linearly dependent?

$$(1,1,1), (1,-1,1), (1,0,-1)$$

no

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

$$(i,1), (1+i, 1-i)$$

yes

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

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

See `mmpc1.mw`

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:

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

Notation: $u^{\mathsf{T}}v$, $u^{\mathsf{T}} \cdot v$, $u^{\dagger}v$,[a] (u, v), $\langle u, v\rangle$, $\vec{u} \cdot \vec{v}$, $\mathbf{u} \cdot \mathbf{v}$, $\langle u|v\rangle$ (bra-ket);
also as a linear form (see below), $u_i v^i$
$\cdot$ = sum over a pair of indices, usually in $\mathbb{R}$

if $(u, v) = 0$, vectors u, v are **perpendicular**

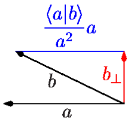
$(u,u)^{1/2} = |u| = ||u||$ = norm[b]

[a] † = transpose + complex conjugate = adjoint = Hermitean (Hermitian) conjugate

[b] 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

For nonzero a, b (zero cases are trivial):[c]



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

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

Pythagoras[d]

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

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

$\Rightarrow$ **triangle inequality**

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

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

[c] Common shortcut: $a^2 \equiv |a^2| = \langle a|a\rangle$

[d] In $\mathbb{C}$, we must be careful because of $\langle b|a\rangle^* = \langle a|b\rangle$; particularly, $|\langle a|b\rangle a|^2 = \langle\langle a|b\rangle^* a|\langle a|b\rangle a\rangle = \langle\langle b|a\rangle a|\langle a|b\rangle a\rangle = |\langle a|b\rangle|^2 a^2$

Hilbert space

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

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

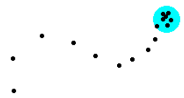
Loosely: "it is not too big",
"there are no problems with using infinite sums"

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. The scalar product is:

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

In chemistry $\boldsymbol{\tau} \in \mathbb{R}^{3n}$, n = # of electrons; there are 2^n-tuples of functions if spin is included



[e] $\{v_i\}_{i=1}^{\infty}$ is Cauchy if $\forall d > 0 \; \exists n : |v_j - v_i| < d \; \forall i, j > n$

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:

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

Scalar product:

$$u \cdot v = \sum u_i v_i \quad \left(\sum u_i^* v_i \text{ in } \mathbb{C} \text{ in physics}\right)$$

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 a 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 $b^{(1)} = (1, i)/\sqrt{2}$.

$(1, -i)c$ for $|c| = 1/\sqrt{2}$

Gram–Schmidt orthogonalization examples: `mmpc1.mw`

Linear forms

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

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

In infinite-dimension spaces there may be continuity problems.
Otherwise in Hilbert spaces linear form $\approx$ scalar product:

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

A linear form (in Euclidean spaces) is also called **covector**:
vector = column vector
covector = row vector (transposed) f^{T}.

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

Covector example

Example. Plane in 3D including the origin can be written as:

$$\vec{n}\cdot\vec{r} = 0,$$

where $\vec{n}$ is perpendicular to the plane = covector.

Maple

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

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
$$x_i \to \sum_{ij} x_i A_{ij} x_j \quad \text{or} \quad x \to x^{\mathsf{T}}\cdot A\cdot x \quad \text{or} \quad x \to x^{\mathsf{T}}Ax \quad \text{or} \quad |x\rangle \to \langle x|\hat{A}|x\rangle$$
- a quadratic tensor; e.g., of pressure

Matrices

Notation:

- In quantum theory often denoted as $\hat{A}$
- $A\cdot x$ 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") must 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**, $A\cdot A^{-1} = A^{-1}\cdot A = \delta$, where $\delta = \mathrm{diag}(1, 1, \ldots)$ = unit matrix (Kronecker delta), also written as E, $\mathbb{1}$, $\boldsymbol{I}$, I, $\overleftrightarrow{I}$, etc.

Determinant

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

$$\det A = \sum_p \mathrm{sign}(p) \prod A_{i,p(i)}$$

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

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

It holds

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

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

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

a) 1, b) $(-1)^{n(n-1)/2}$ (= 1 for $n \equiv 0, 3 \bmod 4$ and -1 otherwise)

Unitary matrix

Orthogonal[f] (in $\mathbb{R}$) or **unitary** (in $\mathbb{C}$) 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

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

- columns U_{*j} can be treated as coordinates of an orthonormal basis (in other orthonormal basis), i.e., a (matrix of) unitary transformation
- U is regular: $U^{-1} = U^\dagger$
- in $\mathbb{R}$: $\det U = \pm 1$, in $\mathbb{C}$: $|\det U| = 1$
- 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`

[f] term "orthonormal" is not used