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 $\mathbb{C}$ (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, $\boldsymbol{v}$, $\vec{v}$ (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 $\{1, \cos(x), \cos(2x), \cos(3x), \ldots\}$. Can function $\cos^2(x)$ be expressed in this basis?

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

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:

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

Notation: $u^{\mathsf T}v$, $u^{\mathsf T}\cdot v$, $u^\dagger v$,[b] (u,v), $\langle u,v\rangle$, $\vec{u}\cdot\vec{v}$, $\boldsymbol{u}\cdot\boldsymbol{v}$, $\langle u|v\rangle$ (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

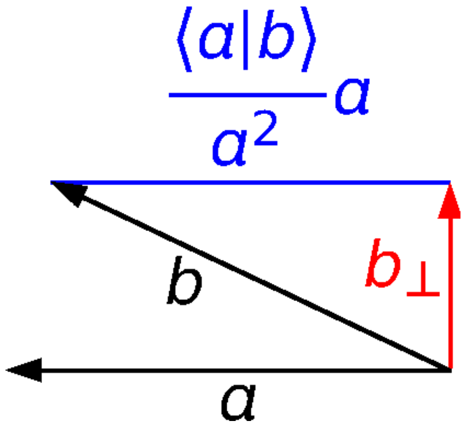
[c]similar space with a norm only (and complete) = Banach space; under some conditions $(u,v)=(|u+v|^2-|u-v|^2)/4$

(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|

⇒ **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:

- 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)

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

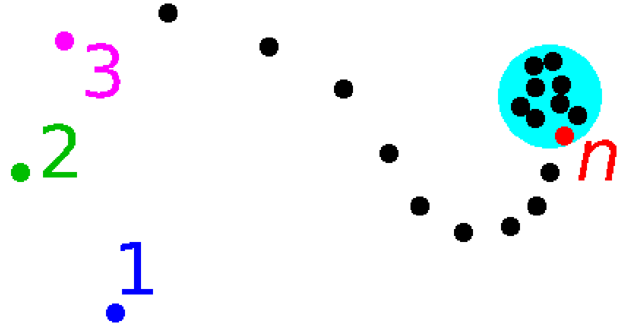
Loosely: ”no vector is missing”
“it is not too big” or “there are no problems with using infinite sums”

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 $\forall d > 0 \; \exists n : |v_j - v_i| < d \; \forall i, j > n$. $\to$ $\to$ $\to$
[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:

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

Scalar product:

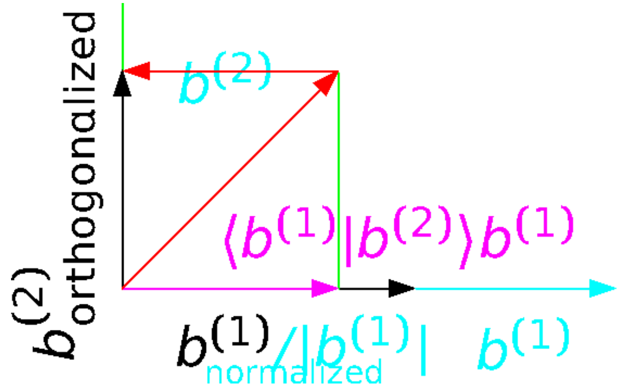
$$u \cdot v = \sum u_i v_i$$

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:



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

":=" 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 $b^{(1)} = (1, i)/\sqrt{2}$ ($b^{(1)}_1 = 1$, $b^{(1)}_2 = i$)

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

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:

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

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^{T}, inverse transformation if a basis changes

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

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

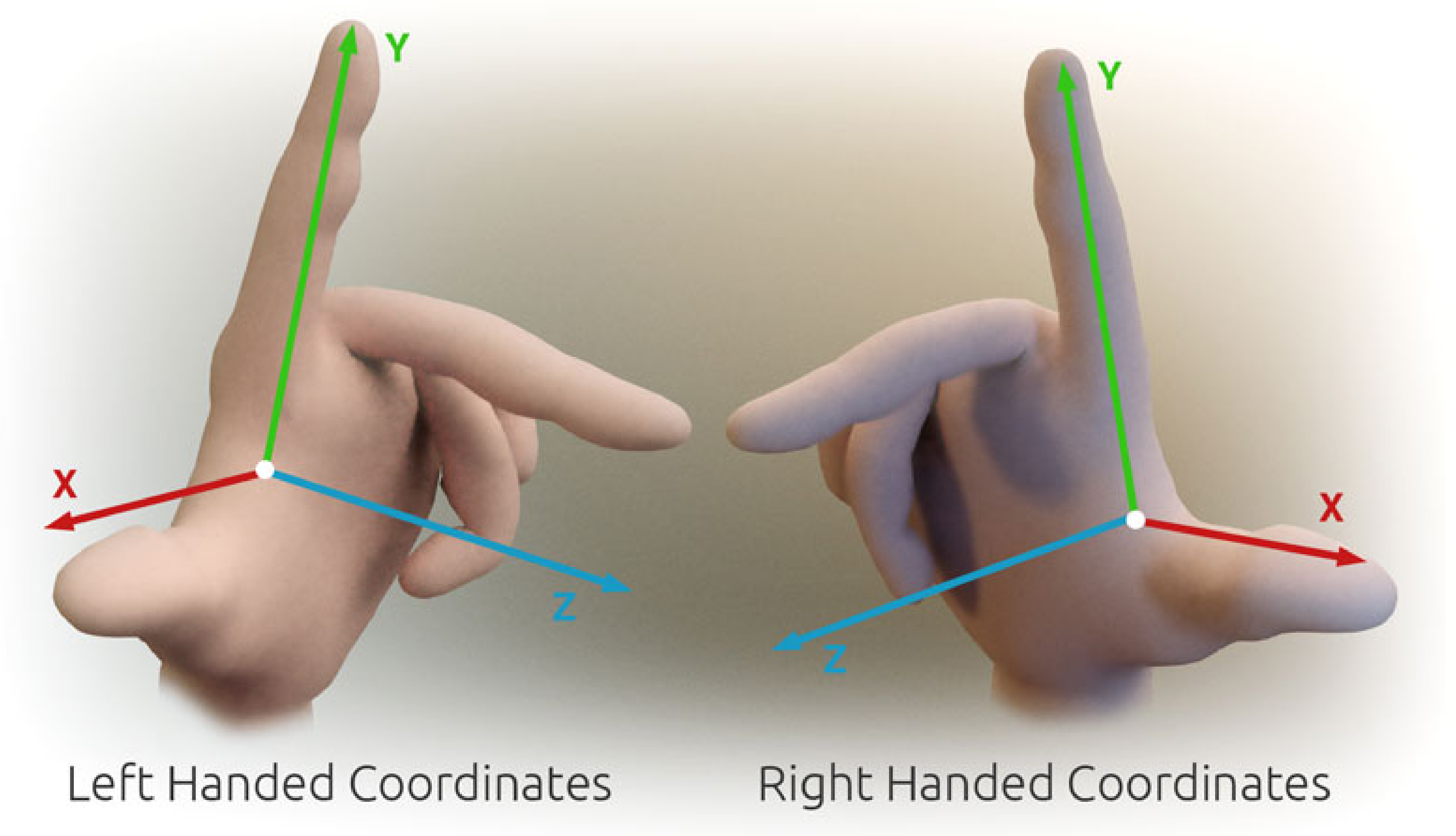
Units: $[\vec{F}]$ = energy/length, $[\mathrm{d}\vec{s}]$ = length.

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

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



credit: Wikipedia

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 $\mathbb{C}^n \to \mathbb{C}$

$$x_i \to \sum_{ij} x_i A_{ij} x_j \quad \text{or} \quad x \to x^{\mathrm{T}} \cdot A \cdot x \quad \text{or} \quad x \to x^{\mathrm{T}} A x \quad \text{or} \quad |x\rangle \to \langle x|\hat{A}|x\rangle$$

- a quadratic tensor; e.g., of pressure or small deformation

Matrices

Notation:

- In quantum theory often denoted as $\hat{A}$
- Other habits (e.g., as tensors): $\overleftrightarrow{A}$, $\underline{\underline{A}}$
- $A \cdot x$ 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 $\delta = \mathrm{diag}(1, 1, \ldots)$ = **unit matrix**, identity matrix, in coordinates Kronecker delta, also written as E, $\mathbb{1}$, $\boldsymbol{I}$, I, $\overleftrightarrow{I}$, etc.

Examples. Invert matrices:

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

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

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 of the 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[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

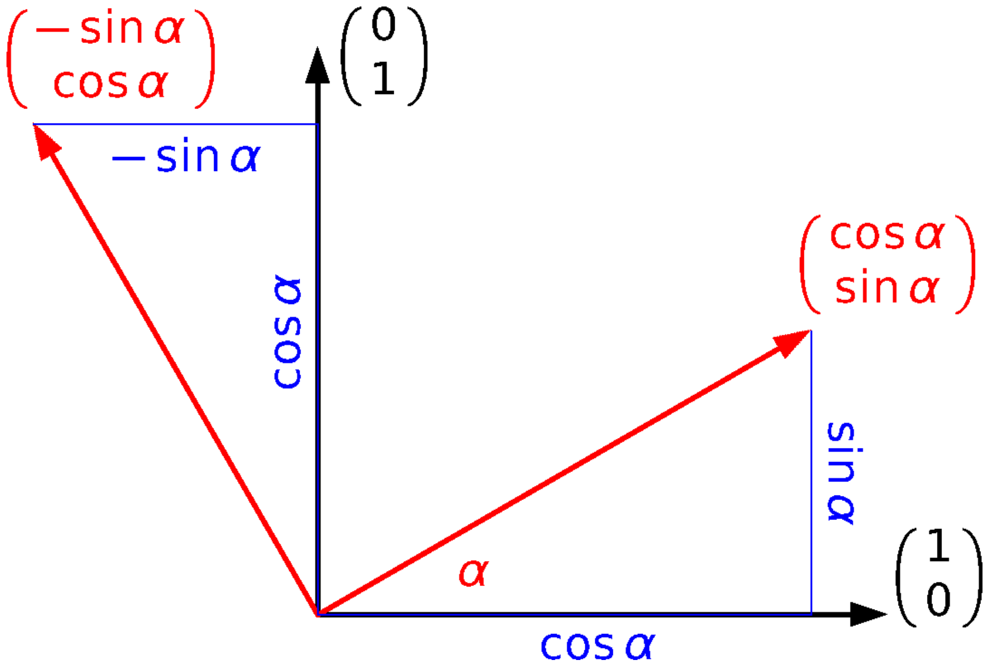
Matrix of rotation

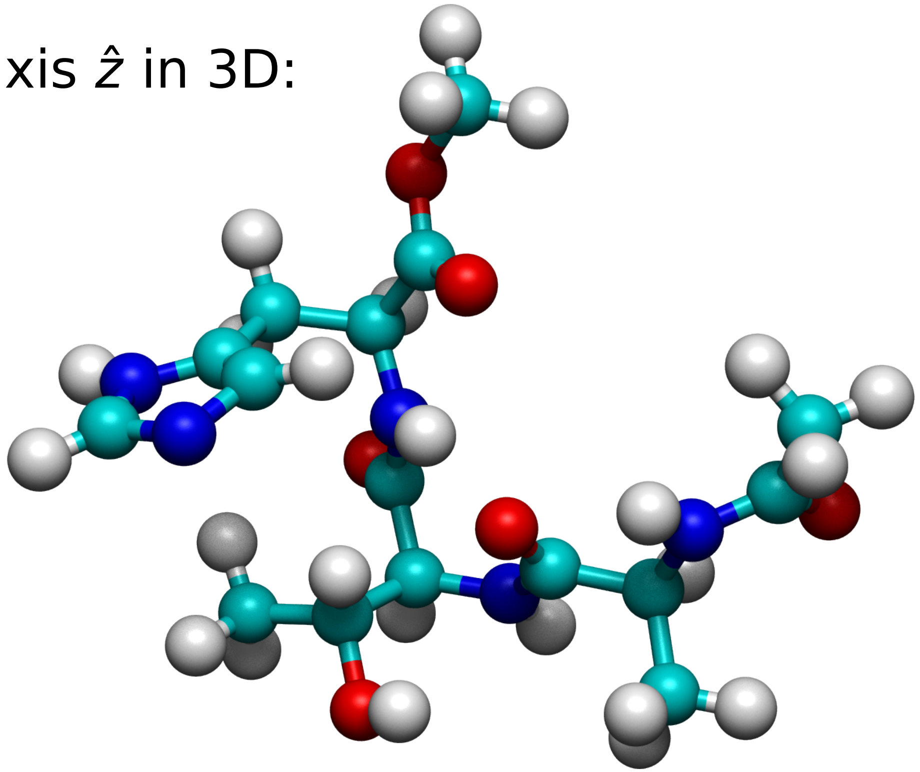
Matrix of rotation by oriented angle $+\alpha$ in 2D:

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

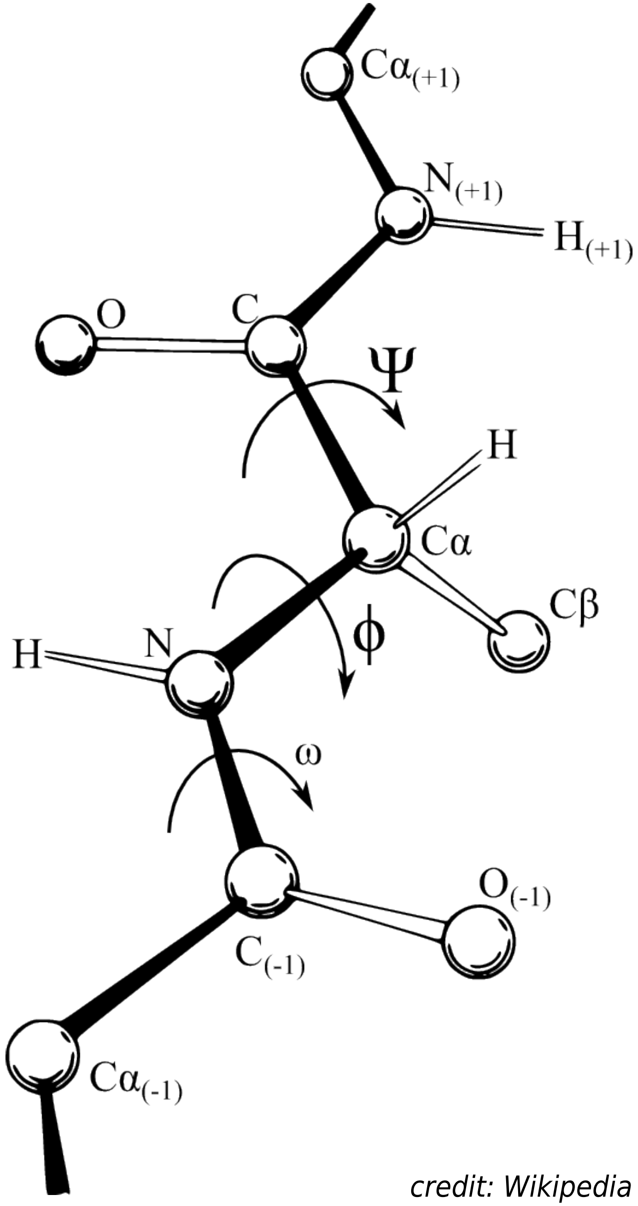
Matrix of rotation by angle α around axis $\hat{z}$ in 3D:

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





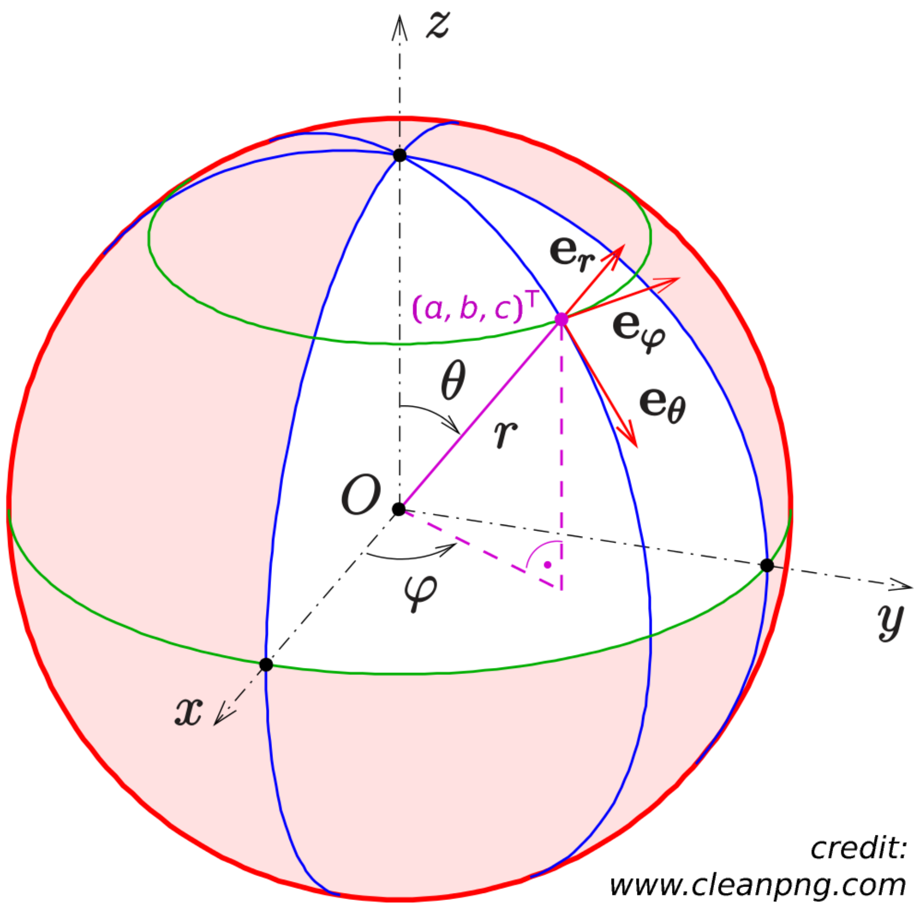
Internal coordinates:



credit: Wikipedia

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

see mmpc1.mw

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