Linear Algebra for Quantum

Disclaimer: Work in progress. Portions of these written materials are incomplete.

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Looking Ahead

Session 1
Vectors and Matrices *basic*

Session 2
Tensor Products *intermediate*

Session 3
Eigenvectors and Eigenvalues *intermediate*

Session 1

- Complex Numbers
- Vectors
  - Bases
  - Linear combinations
  - Bra-ket notation
- Matrices
  - Rank
  - Matrix multiplication
  - Unitary operators

Complex Numbers

a brief review

A **complex number** is of the following form:

$i = \sqrt{-1}$

"imaginary part"

$$z = x + iy$$

"real part"

$i^2 = -1$

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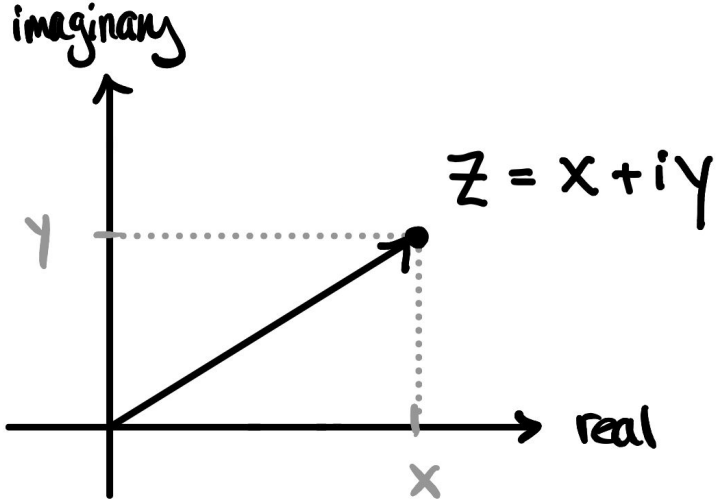

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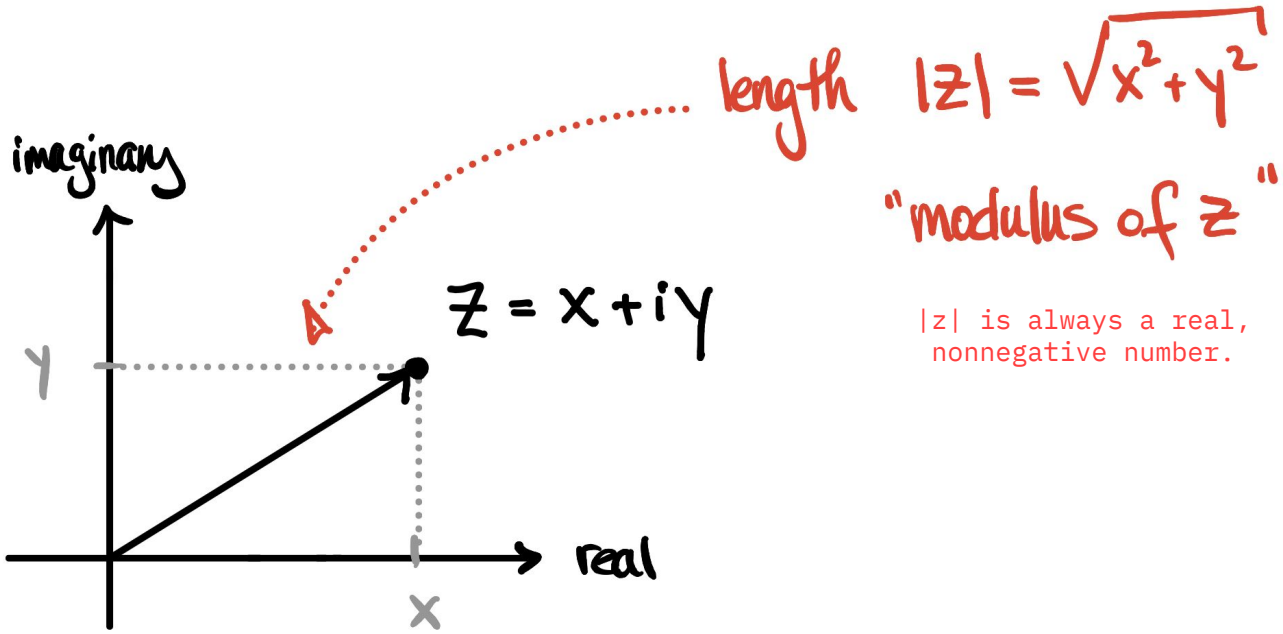

|z| is always a real, nonnegative number.

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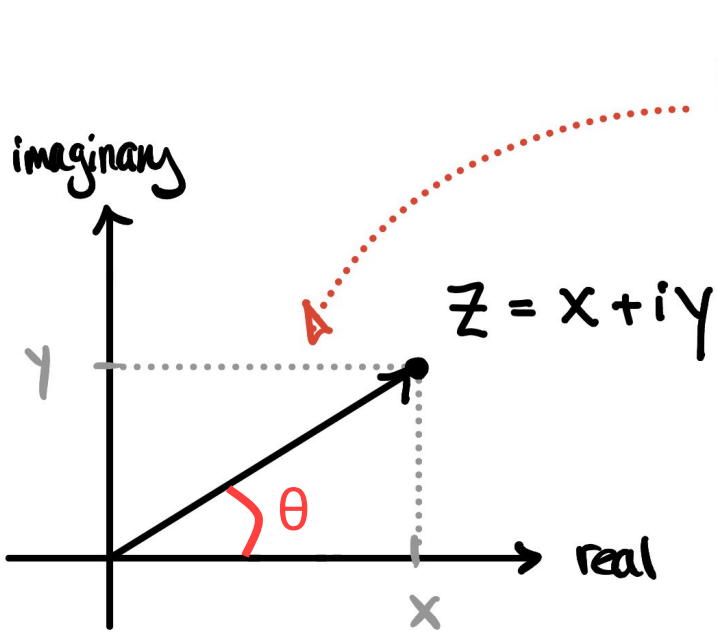
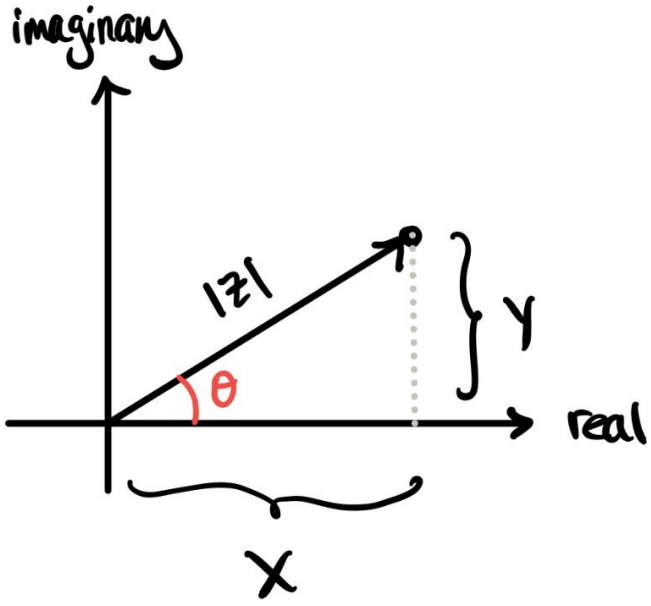


length $|z| = \sqrt{x^2+y^2}$

"modulus of z"

$$\boxed{z = |z|\, e^{i\theta}}$$

Why? Recall from trigonometry:



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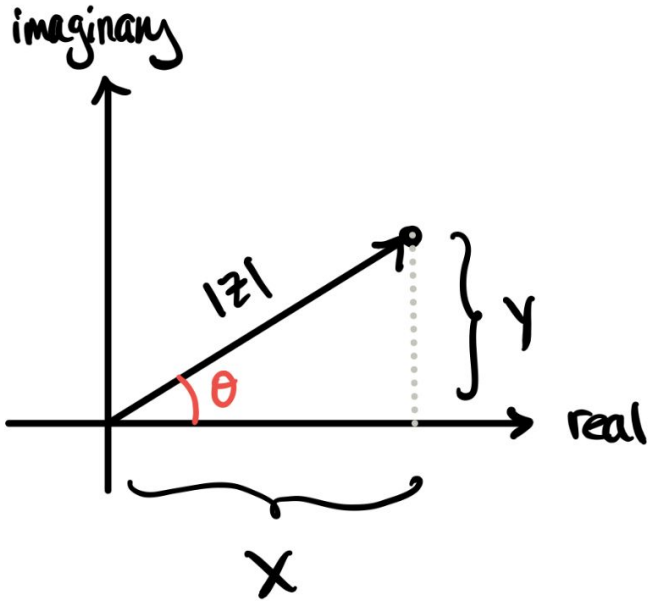

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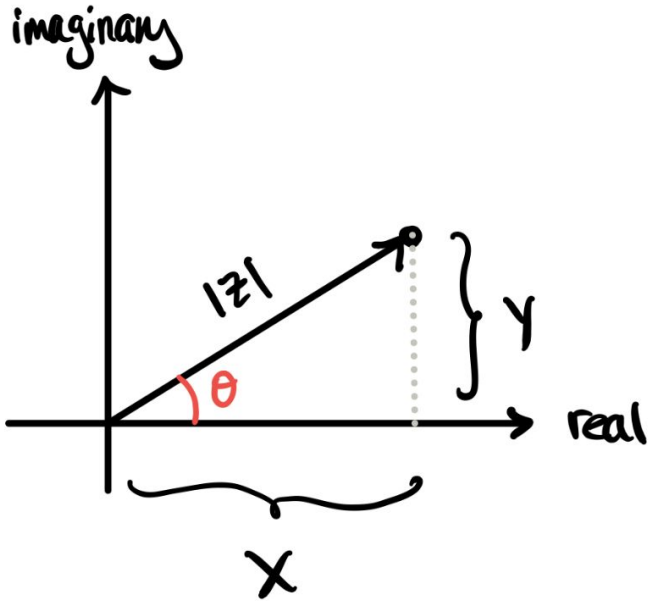

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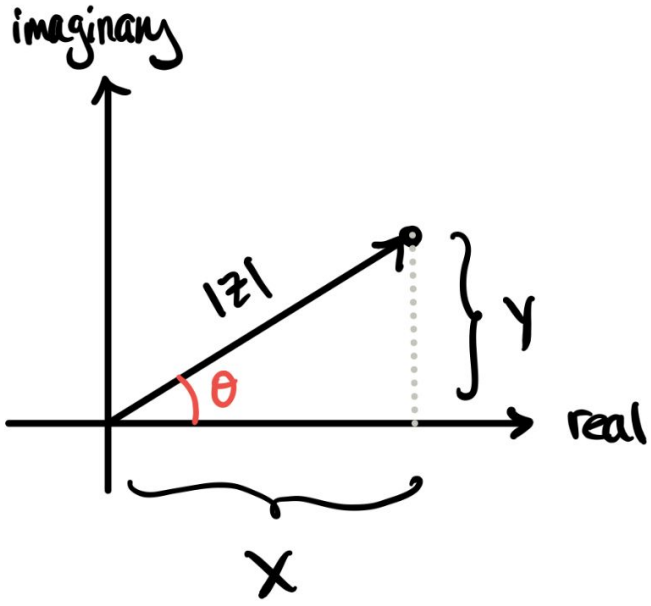

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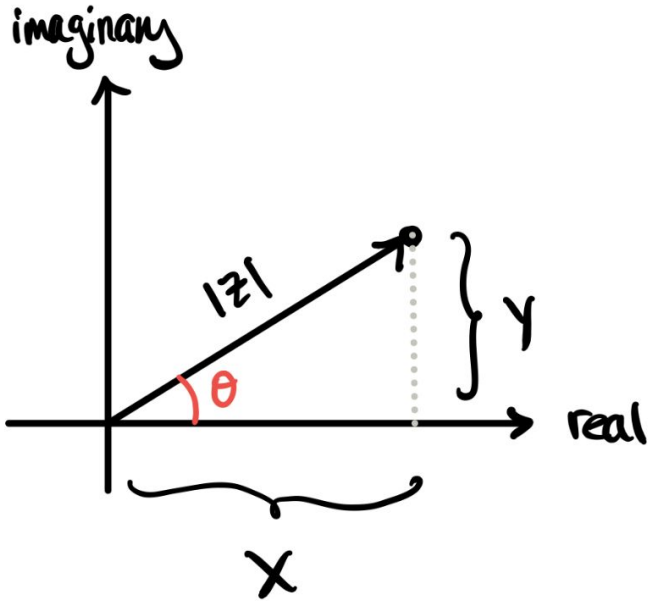

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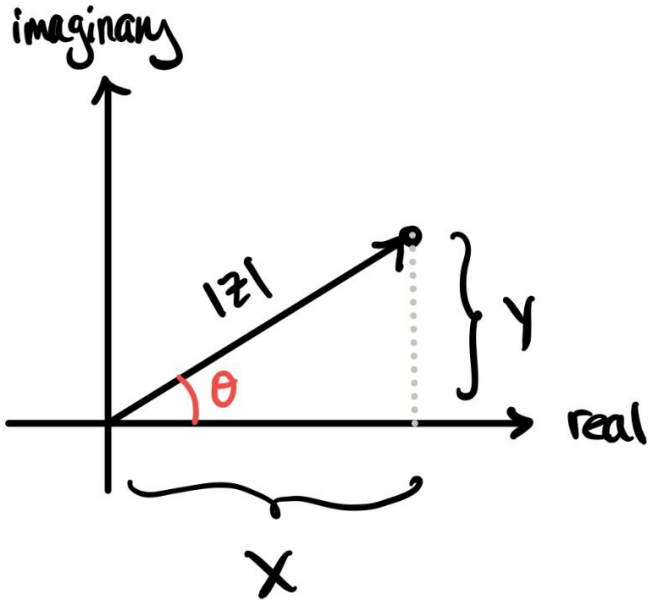


$x = |z|\cos\theta$ $\qquad$ $y = |z|\sin\theta$

$$z = x + iy = |z|(\cos\theta + i\sin\theta)$$

$$= |z|\, e^{i\theta}$$

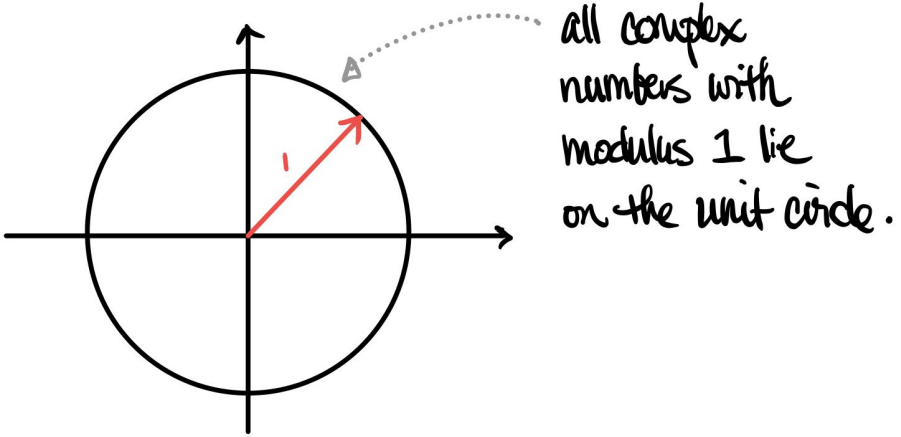
Other things to know:

The "modulus" of z is $|z|$.

The "conjugate" of z is $\bar{z} = x - iy$.

$$\boxed{z\bar{z} = |z|^2}$$

(exercise)



Exercises

1. If $z_1 = |z_1| e^{i\theta_1}$ and $z_2 = |z_2| e^{i\theta_2}$, prove that

$$z_1 z_2 = |z_1| \cdot |z_2| \, e^{i(\theta_1 + \theta_2)}$$

angles add

lengths multiply

2. Show that multiplying $z = |z| e^{i\theta}$ by a phase $e^{i\theta'}$ rotates z by the angle θ'.

3. Show that complex conjugation $z \mapsto \bar{z}$ corresponds to reflection across the real axis.

Vectors

a brief review

The basics.

A **vector** is often thought of as an arrow with a length and a direction.

It can be represented as a 1D array of numbers.

(There's a more abstract way to describe vectors, which we'll omit.)

$$v = \quad = \begin{bmatrix} -3 \\ 0.7 \\ 2 \end{bmatrix}$$

Vectors can be **added** and **subtracted** and **multiplied** by numbers.

Each of these operations is performed entry-wise.

$$v = \begin{bmatrix} 7i \\ 0 \end{bmatrix} \qquad w = \begin{bmatrix} -1 \\ 2+3i \end{bmatrix}$$

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add

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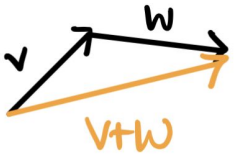

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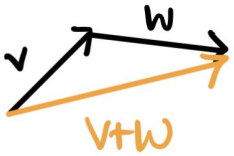
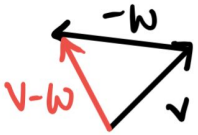
add

subtract

$$v + w = \begin{bmatrix} -1+7i \\ 2+3i \end{bmatrix} \qquad v - w = \begin{bmatrix} 1+7i \\ 2+3i \end{bmatrix}$$





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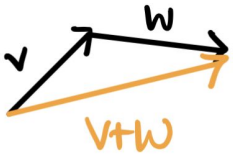
$$v = \begin{bmatrix} 7i \\ 0 \end{bmatrix} \qquad w = \begin{bmatrix} -1 \\ 2+3i \end{bmatrix}$$

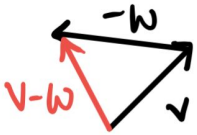
add

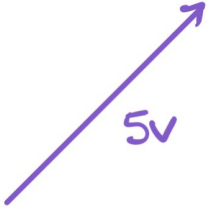
subtract

scalar multiply

$$v + w = \begin{bmatrix} -1+7i \\ 2+3i \end{bmatrix} \qquad v - w = \begin{bmatrix} 1+7i \\ 2+3i \end{bmatrix} \qquad 5v = \begin{bmatrix} 35i \\ 0 \end{bmatrix}$$







The totality of all vectors with n entries is call an ***n*-dimensional** [blank] **vector space**. The adjective “blank” depends on whether the entries are *real* or *complex* numbers.

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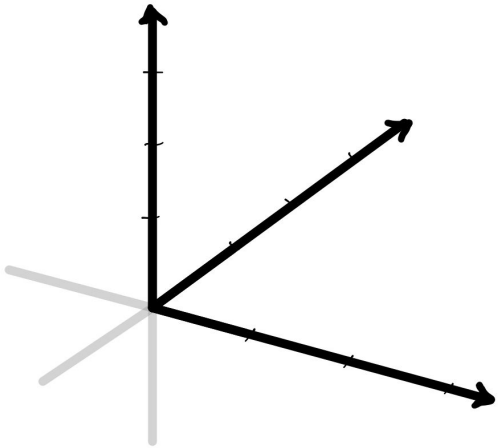
$\mathbb{R}^3$

3-dimensional real vector space

$$\begin{bmatrix} 7 \\ 0.2 \\ 4 \end{bmatrix}$$



This is a "picture" of $\mathbb{R}^3$ not of $\mathbb{C}^3$, which would take 6 dimensions to visualize!

$\mathbb{C}^3$

3-dimensional complex vector space

$$\begin{bmatrix} 3i \\ 0 \\ -2+7i \end{bmatrix}$$

In either case, some vectors play an especially important role: they are called **basis vectors** and are the building blocks for all other vectors.

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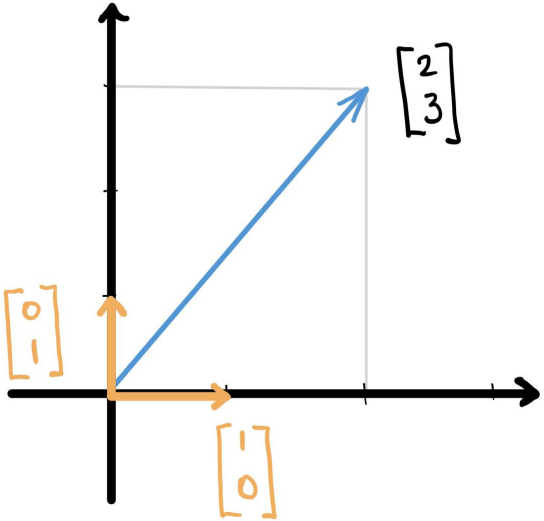
$$\begin{bmatrix} 2 \\ 3 \end{bmatrix} = 2\underline{\underline{\begin{bmatrix} 1 \\ 0 \end{bmatrix}}} + 3\underline{\underline{\begin{bmatrix} 0 \\ 1 \end{bmatrix}}}$$

basis vectors in 2-dimensional space



More generally, every vector with n entries is a “weighted sum” of n basis vectors. The number of basis vectors is called the **dimension** of the vector space.

$$v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix} = v_1 \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + v_2 \begin{bmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + \cdots + v_n \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$$

these can be real or complex numbers

A “weighted sum” of vectors is called a **linear combination** (or *superposition)* and the weights are called **coefficients.**

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"coefficients"

If $w = 3\begin{bmatrix} * \\ * \\ * \end{bmatrix} - 7i\begin{bmatrix} * \\ * \\ * \end{bmatrix} + 5\begin{bmatrix} * \\ * \\ * \end{bmatrix}$, then

w is a "linear combination" of three vectors.

Interlude: Better Notation

In the context of physics, it’s helpful to use **bra-ket** notation:

before:

$$v = \begin{bmatrix} 2i \\ 7 \end{bmatrix}$$

after:

$$|v\rangle = \begin{bmatrix} 2i \\ 7 \end{bmatrix}$$

a "ket"

Let's write **basis vectors** in ket notation, too.
For each $i = 0,...,n-1$ let $|i\rangle$ denote the n-dimensional basis vector with a 1 in the ith entry and 0s elsewhere.

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$\vdots$

A basis for $\mathbb{C}^n$ is $|0\rangle = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$ and $\ldots$ $|n-1\rangle = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}$.

$$|i\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

i^{th} basis vector

$$|i\rangle = \begin{bmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix} \rightsquigarrow |v\rangle = \sum_{i=0}^{n-1} v_i |i\rangle = \begin{bmatrix} v_0 \\ v_1 \\ \vdots \\ v_{n-1} \end{bmatrix}$$

i^{th} basis vector

arbitrary vector in $\mathbb{C}^n$

So a “ket” is just a vector. Here’s another definition.

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The <u>conjugate transpose</u> of $|v\rangle = \begin{bmatrix} 2i \\ 7 \end{bmatrix}$ is

$$(|v\rangle)^{\dagger} = \langle v| = \begin{bmatrix} -2i & 7 \end{bmatrix}$$

"bra"

take the complex conjugate of each entry & "transpose" the array.

$$(|v\rangle)^{\dagger} =$$

conjugate
transpose

$$(|v\rangle)^{\dagger} = \sum_{i=0}^{n-1} \overline{v_i} \langle i|$$

conjugate transpose

$$[0 \cdots 1 \cdots 0]$$

i^{th} spot

$$(|v\rangle)^{\dagger} = \sum_{i=0}^{n-1} \overline{v_i} \langle i| \overset{\text{def.}}{=} \langle v|$$

conjugate transpose

$$[0 \cdots 1 \cdots 0]$$

i^{th} spot

bra

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$$= \boxed{8-7i}$$

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More generally, if $|v\rangle = \sum_{i=0}^{n-1} v_i |i\rangle$ and $|w\rangle = \sum_{i=0}^{n-1} w_i |i\rangle$,

$$\boxed{\langle v | w \rangle = \sum_{i=0}^{n-1} \bar{v}_i w_i}$$

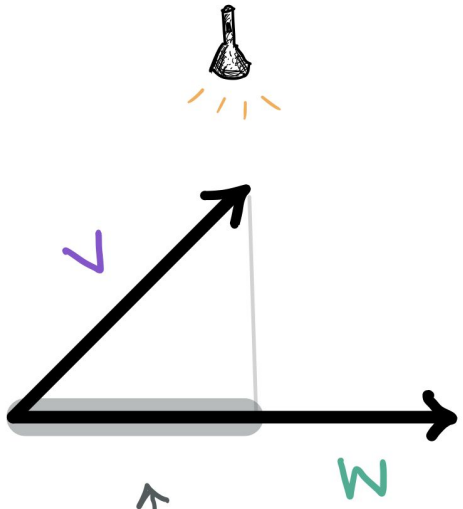
"the **inner product** of |v⟩ and |w⟩"

What's the intuition?

In real vector spaces, this **inner product** represents the length of the "shadow" of one vector along another.

This indicates how similar the vectors are. (E.g. "cosine similarity" between vector embeddings in ML.)

Follows from trigonometry.



length of shadow is $\langle v | w \rangle$ (if length of w is 1)

A couple more definitions

(motivated by a remark)

Remark: This is just *one* example of an inner product, which has a formal definition. Integration is another example.

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A finite-dimensional vector space *together with* an inner product is called a **Hilbert space**.*

*A **Hilbert space** has a more technical definition, but it reduces to this simple statement for finite-dimensional vector spaces.

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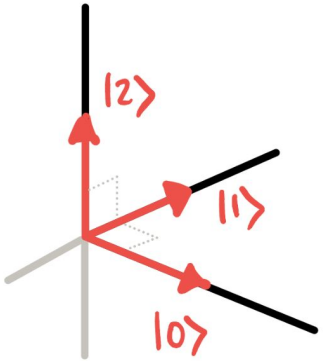
The basis vectors $\{|0\rangle, |1\rangle, \ldots, |n-1\rangle\}$ are <u>orthonormal</u>.

$$\langle i|j\rangle = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{else} \end{cases}$$



Intuitively, orthogonal vectors point in **perpendicular** directions, and further having length 1 means they're "**easy**" to work with (no extra numbers to carry around). The formal definition of *magnitude* is given in the exercises.

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by "linearity"

$$= \sum_{j=0}^{n-1} \langle i|v_j|j\rangle$$

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We'll see more examples later.

If $|v\rangle = \sum_{j=0}^{n-1} v_j |j\rangle$, then

$$\begin{aligned}
\langle i|v\rangle &= \langle i| \sum_{j=0}^{n-1} v_j |j\rangle \\
&= \sum_{j=0}^{n-1} \langle i| v_j |j\rangle \\
&= \sum_{j=0}^{n-1} v_j \langle i|j\rangle \\
&= v_i
\end{aligned}$$

by "linearity"

by "linearity"

by orthonormality

Exercises

Below, let $|v\rangle = \sum_{i=0}^{n-1} v_i |i\rangle$ and $|w\rangle = \sum_{i=0}^{n-1} w_i |i\rangle$ be vectors in an n-dimensional complex vector space.

$\boxed{1}$ Show that $\overline{\langle v|w\rangle} = \langle w|v\rangle$.

$\boxed{2}$ The <u>magnitude</u> (or length) of $|v\rangle$ is defined to be

$$\|v\| = \sqrt{\sum_{i=0}^{n-1} \bar{v}_i v_i}.$$ Prove that $\langle v|v\rangle = \|v\|^2$.

* $\boxed{3}$ A vector whose magnitude is 1 is called a unit vector. Show that every unit vector in $\mathbb{C}^n$ defines a probability distribution on the set $\{0, 1, \ldots, n-1\}$.

Break

(5 min.)

Solution Walk-Through

(5 min.)

Solution #3.

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The $v_i \in \mathbb{C}$ are "probability amplitudes." The $|v_i|^2 \in \mathbb{R}$ are probabilities.

Break

(5 min.)

Matrices

a brief review

A **matrix** is a 2-dimensional array of (real or complex) numbers.

It represents a **process** of turning one vector into another: stretching, rotating, scaling, or something more involved.

$$\begin{bmatrix} 3 & 0 & 7 \\ 1 & -5 & 9 \\ 2 & 0 & 0 \end{bmatrix} \underbrace{\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}}_{\text{input}} = \underbrace{\begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}}_{\text{output}}$$

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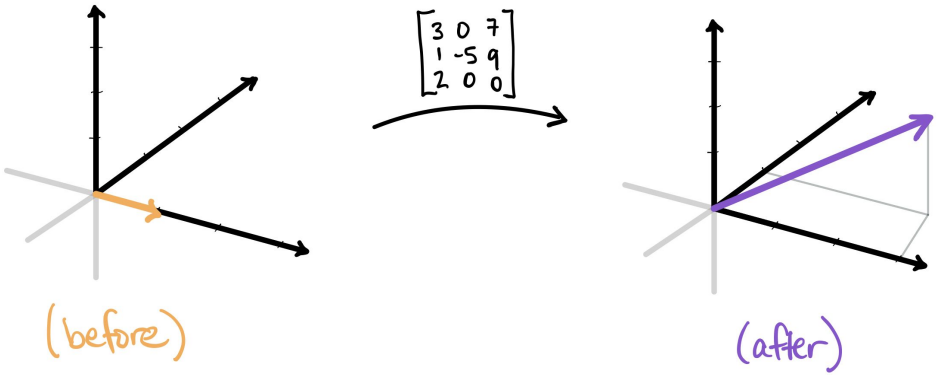
It represents a **process** of turning one vector into another: stretching, rotating, scaling, or something more involved.

Better: it represents a **linear transformation** of an *entire* vector space to another (possibly of different dimensions).



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3 1 2

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The matrix $|v\rangle\langle w|$ is called the **outer product** of $|v\rangle$ and $|w\rangle$, in contrast to their **inner product** $\langle v|w\rangle$.

If $|0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$ and $|2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ then

$$|0\rangle\langle 2| = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

a 1 in the 0th row, 2nd column and zeros elsewhere

More generally, $|i\rangle\langle j| =$

$$\begin{array}{cc} & j^{th}\ \text{col} \\ i^{th}\ \text{row} & \begin{bmatrix} & \vdots & \\ \cdots & 1 & \\ & & \end{bmatrix} \end{array}$$

With this, the entries of any matrix can be expressed in bra-ket notation:

$$M = \begin{bmatrix} m_{00} & m_{01} & m_{02} \\ m_{10} & m_{11} & m_{12} \\ m_{20} & m_{21} & m_{22} \end{bmatrix}$$

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$$\xRightarrow{\text{exercise}} \quad \boxed{m_{ij} = \langle i | M | j \rangle}$$

Let’s do one more?

Here’s what **matrix-vector multiplication** looks like in bra-ket notation:

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Here's what **matrix-vector multiplication** looks like in bra-ket notation:

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if $M = \sum_{i,j} m_{ij} |i\rangle\langle j|$ and $|v\rangle = \sum_k v_k |k\rangle$ then

$$M|v\rangle = \sum_{i,j,k} m_{ij} |i\rangle\langle j|v_k|k\rangle$$

linearity

$$= \sum_{i,j,k} m_{ij} v_k |i\rangle\langle j|k\rangle$$

orthonormality

$$= \sum_{i,j} m_{ij} v_j |i\rangle$$

$$M|v\rangle = \begin{bmatrix} \vdots \\ * \\ \vdots \end{bmatrix}$$

ith entry of $M|v\rangle$ is $\sum_j m_{ij} v_j$

What is “linearity” anyway?

A function between vector spaces $T: V \longrightarrow V'$ is called a **linear transformation** if it satisfies the following:

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(1) $$T(|v\rangle + |w\rangle) = T(|v\rangle) + T(|w\rangle)$$

(2) $$T(\alpha|v\rangle) = \alpha T(|v\rangle)$$

any number

(1) says that adding two vectors and then applying T is the same as first applying T and then adding the results.
(2) says that scaling a vector and then applying T is the same as first applying T and then scaling the result.

Non-Example

The function $T: \mathbb{R}^2 \to \mathbb{R}^2$ defined by $T\left(\begin{bmatrix} a \\ b \end{bmatrix}\right) = \begin{bmatrix} a^2 \\ b \end{bmatrix}$

is <u>NOT LINEAR</u>!

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Non-Example

$$T\left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} -1 \\ 0 \end{bmatrix}\right) = T\left(\begin{bmatrix} 1-1 \\ 0+0 \end{bmatrix}\right) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

not equal!

$$T\left(\begin{bmatrix} 1 \\ 0 \end{bmatrix}\right) + T\left(\begin{bmatrix} -1 \\ 0 \end{bmatrix}\right) = \begin{bmatrix} 1^2 \\ 0 \end{bmatrix} + \begin{bmatrix} (-1)^2 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

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Every matrix is a linear transformation. Follows from properties of basic arithmetic: commutativity and distributivity.

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matrices $\rightleftarrows$ linear transformations

$$\begin{bmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

$n \times m$

$\mathbb{C}^m \longrightarrow \mathbb{C}^n$

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$$M = \begin{bmatrix} 2i & 3 \\ 1 & 0 \end{bmatrix} \qquad N = \begin{bmatrix} -2i & 9 \\ 5 & 4 \end{bmatrix}$$

add

$$M + N = \begin{bmatrix} 0 & 12 \\ 6 & 4 \end{bmatrix}$$

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add

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scalar multiply

$$M + N = \begin{bmatrix} 0 & 12 \\ 6 & 4 \end{bmatrix} \qquad M - N = \begin{bmatrix} 4i & -6 \\ -4 & -4 \end{bmatrix} \qquad 5M = \begin{bmatrix} 10i & 15 \\ 5 & 0 \end{bmatrix}$$

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Matrices can also be **multiplied together**. The product of matrices represents the *composition* of the linear transformations.

a 2×3 matrix

a 4×2 matrix

$$\begin{tikzcd} \mathbb{R}^3 \arrow[r, "M"] \arrow[rr, bend right, dotted] & \mathbb{R}^2 \arrow[r, "N"] & \mathbb{R}^4 \end{tikzcd}$$

$$N \circ M = NM$$

a 4×3 matrix

$$\underset{4\times 3}{NM} = \overset{N}{\underset{4\times 2}{\begin{bmatrix} 0 & 5 \\ 1 & 0 \\ 0 & -3 \\ 0 & 4 \end{bmatrix}}} \overset{M}{\underset{2\times 3}{\begin{bmatrix} 2 & 0 & 0 \\ 1 & 0 & -3 \end{bmatrix}}} =$$

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5

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Exercise:
verify the rest!

Aside

Vectors and matrices can be *much more abstract* than arrays of numbers.

- The space of continuously differentiable functions on $\mathbb{R}$ is a vector space and **differentiation** is a linear transformation on this space.

$$\frac{d}{dx}(f+g) = \frac{df}{dx} + \frac{dg}{dx} \qquad \frac{d}{dx}(kf) = k\frac{df}{dx}$$

- **Integration** is likewise a linear transformation:

$$\int f+g\,dx = \int f\,dx + \int g\,dx \qquad \int kf\,dx = k\int f\,dx$$

Quick (important) definitions

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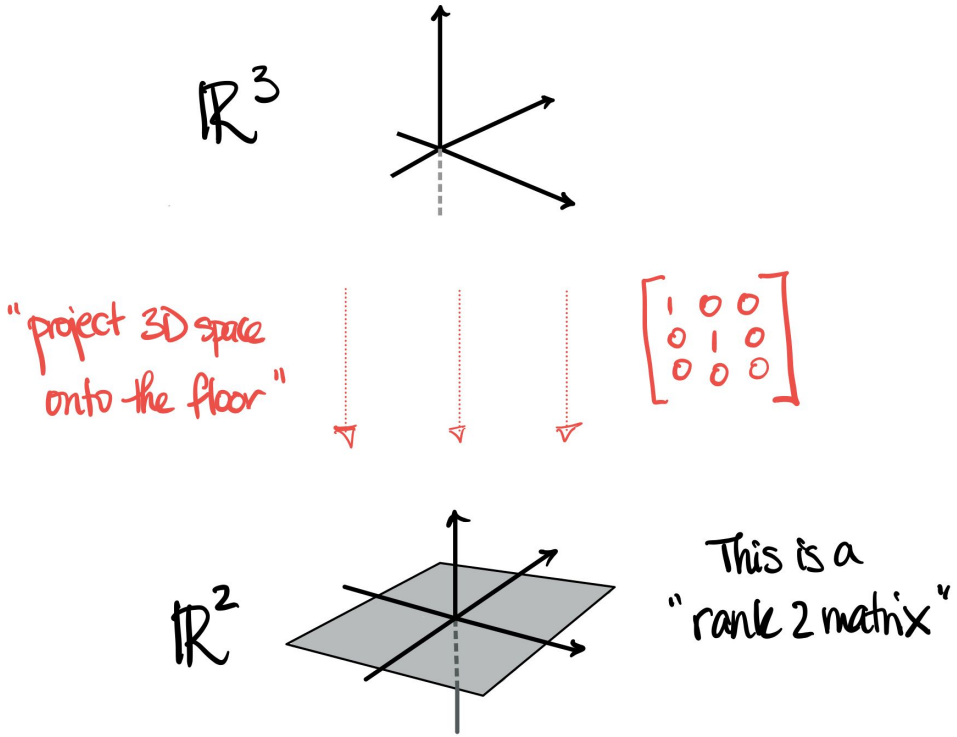

The **transpose** of a matrix M is a matrix M^T whose rows are the columns of M and whose columns are the rows of M.

$$\underset{2\times 3}{M} = \begin{bmatrix} 7 & i & 2 \\ 5 & 0 & 4-3i \end{bmatrix} \longrightarrow \underset{3\times 2}{M^T} = \begin{bmatrix} 7 & 5 \\ i & 0 \\ 2 & 4-3i \end{bmatrix}$$

If M represents a linear transformation $\mathbb{C}^3 \longrightarrow \mathbb{C}^2$ then M^T represents a linear transformation in the other direction, $\mathbb{C}^2 \longrightarrow \mathbb{C}^3$. *Question worth pondering: Does M^T "undo" the transformation made by M?*

The **conjugate transpose** of a matrix M is the matrix $M^\dagger$ obtained by first transposing M then taking the complex conjugate of each entry (or vice versa: verify the order doesn't matter).

$$\underset{2\times 3}{M} = \begin{bmatrix} 7 & i & 2 \\ 5 & 0 & 4-3i \end{bmatrix} \longrightarrow \underset{3\times 2}{M^\dagger} = \begin{bmatrix} 7 & 5 \\ -i & 0 \\ 2 & 4+3i \end{bmatrix}$$

A square matrix M is called **Hermitian** if it is equal to its conjugate transpose, $M = M^\dagger$.

self-adjoint ✓

$$\begin{bmatrix} 1 & 2i & 7 \\ -2i & 0 & 4-i \\ 7 & 4+i & 5 \end{bmatrix}$$

not self-adjoint ✗

$$\begin{bmatrix} 1 & 2i & 7 \\ 3 & 0 & 4-i \\ 0 & -i & 9i \end{bmatrix}$$

Hermitian matrices have a nice symmetry, so they're easy to spot with the eye!

The n×n **identity matrix** is the square matrix I with 1s along the diagonal and 0s elsewhere.

$$I = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \sum_{i=0}^{2} |i\rangle\langle i|$$

It has the property that $I|v\rangle=|v\rangle$ and $IM=MI = M$ for all vectors $|v\rangle$ and for all matrices M. It’s the “do nothing” transformation.

If $|v\rangle = \sum_{j=0}^{2} v_j |j\rangle$, then

$$I|v\rangle = \sum_{i=0}^{2} \sum_{j=0}^{2} |i\rangle\langle i|v_j|j\rangle$$

linearity

$$= \sum_{i=0}^{2} \sum_{j=0}^{2} v_j |i\rangle\langle i|j\rangle$$

orthonormality

$$= \sum_{i=0}^{2} v_i |i\rangle$$

$$= |v\rangle.$$

A, nxn square matrix M is called **invertible** if there exists a matrix M^{-1} such that $MM^{-1} = M^{-1}M = I$, where I is the nxn identity matrix. In this case, M^{-1} is called the **inverse of M**.

$$\begin{tikzcd} \mathbb{C}^n \arrow[r, shift left, dashed, "M"] & \mathbb{C}^n \arrow[l, shift left, dashed, "M^{-1}"] \end{tikzcd}$$

Not all matrices are invertible. But some matrices *are* and for some of those matrices, we know exactly what the inverse is...

An $n \times n$ square matrix U is called **unitary** if it is *invertible* and its inverse is equal to $U^\dagger$.

In other words, unitary matrices satisfy

$$UU^\dagger = U^\dagger U = I$$

where I is the $n \times n$ identity matrix.

The condition $UU^\dagger = U^\dagger U = I$ tells us that the columns (and rows) of U are orthonormal.

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In other words, unitary matrices satisfy

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where I is the n×n identity matrix.

$$U = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -i/\sqrt{2} & i/\sqrt{2} & 0 \\ 0 & 0 & i \end{bmatrix} \qquad U^\dagger = \begin{bmatrix} 1/\sqrt{2} & i/\sqrt{2} & 0 \\ 1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & 0 & -i \end{bmatrix}$$

$$UU^\dagger = U^\dagger U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

3x3 identity matrix

Exercise: verify this computation!

The condition $UU^\dagger = U^\dagger U = I$ tells us that the columns (and rows) of U are orthonormal.

Exercises

1. Is matrix multiplication commutative? In other words, is it true that $MN = NM$ for all square matrices M and N? If so, explain why. If not, why not?

2. a. Find the matrix that represents the linear transformation $T: \mathbb{C}^3 \to \mathbb{C}^3$ defined by:

$$T(|1\rangle) = 5|1\rangle + |2\rangle, \quad T(|2\rangle) = i|3\rangle, \quad T(|3\rangle) = |3\rangle$$

b. Describe the linear transformation $T: \mathbb{C}^3 \to \mathbb{C}^3$ represented by this 3×3 matrix by explaining its assignment on the basis vectors $\{|1\rangle, |2\rangle, |3\rangle\}$ of $\mathbb{C}^3$.

$$\begin{bmatrix} 1-i & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

3. Show that the diagonal entries of a Hermitian matrix must be <u>real</u>, not complex, numbers.

* 4. Show that if $\mathcal{U}$ is an $n\times n$ unitary matrix then $\langle v|w\rangle = \langle \mathcal{U}v|\mathcal{U}w\rangle$ for all $|v\rangle, |w\rangle \in \mathbb{C}^n$. Conclude that unitary matrices preserve the lengths of vectors.

Break

(5 min.)

Solution Walk-Through

(10 min.)

Solution #4.

Suppose $U : \mathbb{C}^n \to \mathbb{C}^n$ is unitary so that $UU^\dagger = U^\dagger U = I$.

$\boxed{\text{Claim}}$:

Solution #4.

Suppose $U : \mathbb{C}^n \to \mathbb{C}^n$ is unitary so that $UU^\dagger = U^\dagger U = I$.

$\boxed{\text{Claim}}$: $\langle Ux | y \rangle = \langle x | U^\dagger y \rangle$ for all $|x\rangle, |y\rangle \in \mathbb{C}^n$.

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suppose for now the claim is true. Then,

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Suppose for now the claim is true. Then,

$$\langle Uv | Uw \rangle \overset{\text{by the claim}}{=}$$

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Suppose for now the claim is true. Then,

$$\langle Uv | Uw \rangle \overset{\text{by the claim}}{=} \langle v | U^\dagger U w \rangle \overset{\text{because U is unitary}}{=}$$

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$$\langle Uv | Uw \rangle \overset{\text{by the claim}}{=} \langle v | U^\dagger U w \rangle \overset{\text{because U is unitary}}{=} \langle v | I w \rangle \overset{\text{because I is the identity}}{=}$$

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Suppose $U : \mathbb{C}^n \to \mathbb{C}^n$ is unitary so that $UU^\dagger = U^\dagger U = I$.

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Suppose for now the claim is true. Then,

$$\langle Uv | Uw \rangle \overset{\text{by the claim}}{=} \langle v | U^\dagger U w \rangle \overset{\text{because U is unitary}}{=} \langle v | I w \rangle \overset{\text{because I is the identity}}{=} \langle v | w \rangle.$$

Solution #4.

In particular if $|w\rangle = |v\rangle$ then

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In particular if $|w\rangle = |v\rangle$ then

$$\|v\|^2 = \langle v|v\rangle = \langle Uv|Uv\rangle = \|Uv\|^2$$

and so unitary matrices preserve lengths of vectors:

$$\boxed{\|Uv\| = \|v\|.}$$

Take the square root of each side above.

Solution #4.

In particular if $|w\rangle = |v\rangle$ then

$$\|v\|^2 = \langle v|v\rangle = \langle Uv|Uv\rangle = \|Uv\|^2$$

and so unitary matrices preserve lengths of vectors:

$$\boxed{\|Uv\| = \|v\|.}$$

Take the square root of each side above.

In particular, they send unit vectors to unit vectors!

i.e. unitaries send probability distributions to probability distributions.

Proof of Claim

$$\langle Ux | y \rangle = \langle x | U^\dagger y \rangle$$

for all vectors $|x\rangle, |y\rangle \in \mathbb{C}^n$.

$$U = \sum_{i,j} U_{ij} |i\rangle\langle j|$$

$$|x\rangle = \sum_k x_k |k\rangle \qquad |y\rangle = \sum_\ell y_\ell |\ell\rangle$$

Notice this claim holds true for **all** matrices, not just unitaries! (The proof doesn't need any assumptions about unitarity.)

Recall from earlier that $U|x\rangle = \sum_{i,j} U_{ij} x_j |i\rangle =$ "$|Ux\rangle$"

and so $\langle Ux| = \sum_{i,j} \overline{U_{ij}}\, \overline{x_j} \langle i|$. Now "plug & chug":

$$\langle Ux | y \rangle = \sum_{i,j} \overline{U_{ij}}\, \overline{x_j} \langle i| \sum_k y_k |k\rangle$$

linearity

$$= \sum_{i,j,k} \overline{U_{ij}}\, \overline{x_j}\, y_k \langle i|k\rangle$$

orthonormality

$$= \sum_{i,j} \overline{U_{ij}}\, \overline{x_j}\, y_i$$

commutativity

$$= \sum_{i,j} \overline{x_j}\, \overline{U_{ij}}\, y_i$$

definition

$$= \langle x | U^\dagger y \rangle$$

Session 2

- Tensor product of vectors / vector spaces
  - Example
  - Tensor product vs. direct sum
- Tensor product of linear maps
  - Kronecker product
- Tensor network diagram notation
  - Brief introduction

The Tensor Product

a brief introduction

Main Idea

The tensor product is a construction from linear algebra used to model *composite* quantum systems.

Last time:

single system

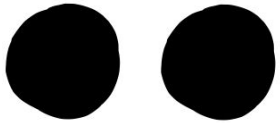
The state of

is a unit vector $|\psi\rangle \in V$.

Hilbert space

Today:

composite system

The state of 

is a unit vector $|\psi\rangle \in V \otimes V$.

the **tensor product** of Hilbert spaces

Today:

composite system

The state of ● ● ... ●

is a unit vector $|\psi\rangle \in V \otimes V \otimes \cdots \otimes V$

the **tensor product** of Hilbert spaces

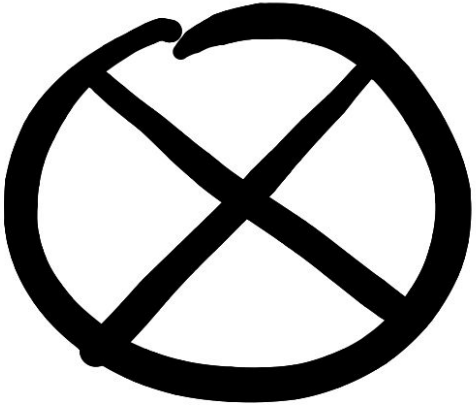
The **tensor product** of vector spaces V and W is *another* vector space, denoted $V \otimes W$.

Q1: What do vectors in the space $V \otimes W$ "look like"?

- Involves the tensor product of *vectors*.

Q2: What is the dimension of $V \otimes W$?

- It's the product of the dimensions of V and W. (Clear after answering Q1.)



Example

To form the **tensor product** of two coordinate vectors, simply “multiply their entries in every way possible.”

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \otimes \begin{bmatrix} 4 \\ 5 \end{bmatrix}$$

$$|v\rangle \otimes |w\rangle$$

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \otimes \begin{bmatrix} 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 1 \cdot 4 \\ 1 \cdot 5 \\ \\ \\ \\ \\ \end{bmatrix}$$

$$|v\rangle \otimes |w\rangle$$

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$$|v\rangle \otimes |w\rangle$$

$$\begin{bmatrix}1\\2\\3\end{bmatrix} \otimes \begin{bmatrix}4\\5\end{bmatrix} = \begin{bmatrix}1\\2\\3\end{bmatrix}\begin{bmatrix}4\\5\end{bmatrix} = \underbrace{\begin{bmatrix}1\cdot 4\\1\cdot 5\\2\cdot 4\\2\cdot 5\\3\cdot 4\\3\cdot 5\end{bmatrix} = \begin{bmatrix}4\\5\\8\\10\\12\\15\end{bmatrix}}_{\text{in } \mathbb{R}^3 \otimes \mathbb{R}^2 \cong \mathbb{R}^6}$$

$$|v\rangle \otimes |w\rangle$$

Exercise: verify!

$$\begin{bmatrix} 2 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 6 \\ 2 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} -1 \\ 1 \\ -1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 9 \\ 3 \end{bmatrix} = \begin{bmatrix} -1 \\ -9 \\ -3 \\ 1 \\ 9 \\ 3 \\ -1 \\ -9 \\ -3 \end{bmatrix}$$

$$\begin{bmatrix} 5 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \\ 4 \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \\ 20 \\ 1 \\ 0 \\ 4 \end{bmatrix}$$

So, what is the vector space $V \otimes W$?

What do the vectors that comprise $V \otimes W$ “look like”?

Guess

If V and W are vector spaces, then their **tensor product** $V \otimes W$ consists of all vectors of the form

$$|v\rangle \otimes |w\rangle$$

where $|v\rangle$ is a vector in V, and $|w\rangle$ is a vector in W.

nope.

~~If V and W are vector spaces, then their **tensor product** $V \otimes W$ consists of all vectors of the form~~

$$\cancel{|v\rangle \otimes |w\rangle}$$

~~where $|v\rangle$ is a vector in V, and $|w\rangle$ is a vector in W.~~

Remember what a vector space is...

Recall that the n-dimensional vector space $\mathbb{R}^n$ consists of all possible **linear combinations** of the basis vectors $\{|0\rangle, |1\rangle, ..., |n-1\rangle\}$.

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$$\mathbb{R}^n = \left\{ \sum_{i=0}^{n-1} v_i |i\rangle \;\middle|\; v_i \in \mathbb{R} \right\}$$

To specify a vector space, it's enough to say what the bases are.*

*Technically a **vector space** is abstractly defined by a list of axioms, and the existence of a basis is a *theorem* (that's equivalent to the **Axiom of Choice**!). But the basis perspective is sufficient for this series.

$$\mathbb{R}^n = \left\{ \sum_{i=0}^{n-1} v_i |i\rangle \;\middle|\; v_i \in \mathbb{R} \right\}$$

a vector space

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a vector space

What goes here?

$$\mathbb{R}^n \otimes \mathbb{R}^m = \left\{ \sum_{??} c_{??} |???\rangle \;\middle|\; c_{??} \in \mathbb{R} \right\}$$

a *tensor product* of vector spaces

If $\{|0\rangle, \ldots, |n-1\rangle\}$ is a basis for $\mathbb{R}^n$, and

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if $\{|0\rangle, \ldots |m-1\rangle\}$ is a basis for $\mathbb{R}^m$,

then

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if $\{|0\rangle, \ldots |m-1\rangle\}$ is a basis for $\mathbb{R}^m$,

then $\left\{ |i\rangle \otimes |j\rangle \;\middle|\; \begin{array}{l} i=0,\ldots,n-1 \\ j=0,\ldots,m-1 \end{array} \right\}$ is a basis for $\underline{\underline{\mathbb{R}^n \otimes \mathbb{R}^m}}$.

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$$|i\rangle \otimes |j\rangle = |i\rangle|j\rangle = |ij\rangle$$

Recall that the ith basis vector $|i\rangle$ has a 1 in the ith entry and 0s elsewhere. So the symbols $\mathbf{|i\rangle \otimes |j\rangle = |i\rangle|j\rangle = |ij\rangle}$ can be understood using the computation introduced earlier.

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Bases for $\mathbb{C}^2$ are $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and so,

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Bases for $\mathbb{C}^2$ are $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and so,

$$|00\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad |01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \quad |10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \quad |11\rangle = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

bases for $\mathbb{C}^2 \otimes \mathbb{C}^2$

$$\mathbb{R}^n \otimes \mathbb{R}^m = \left\{ \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} c_{ij} \, |ij\rangle \;\middle|\; c_{ij} \in \mathbb{R} \right\}$$

$$\mathbb{R}^n \otimes \mathbb{R}^m = \left\{ \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} c_{ij} |ij\rangle \;\middle|\; c_{ij} \in \mathbb{R} \right\}$$

$$3|00\rangle + 7|10\rangle - \sqrt{2}|11\rangle$$

An example of a vector in $\mathbb{R}^3 \otimes \mathbb{R}^2$.

$$\mathbb{C}^n \otimes \mathbb{C}^m = \left\{ \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} c_{ij} |ij\rangle \;\middle|\; c_{ij} \in \mathbb{C} \right\}$$

$$\mathbb{C}^n \otimes \mathbb{C}^m = \left\{ \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} c_{ij} |ij\rangle \;\middle|\; c_{ij} \in \mathbb{C} \right\}$$

$$3i|00\rangle - 7|10\rangle - (\sqrt{2}+5i)|11\rangle$$

An example of a vector in $\mathbb{C}^3 \otimes \mathbb{C}^2$.

$$\mathbb{C}^n \otimes \mathbb{C}^m = \left\{ \sum_{i=0}^{n-1} \sum_{j=0}^{m-1} c_{ij} |ij\rangle \;\middle|\; c_{ij} \in \mathbb{C} \right\}$$

$$\dim\left(\mathbb{C}^n \otimes \mathbb{C}^m\right) = nm = \dim\left(\mathbb{C}^n\right)\dim\left(\mathbb{C}^m\right)$$

The **dimension** of the tensor product is the *product* of the respective dimensions.

More generally, if V and W are arbitrary vector spaces with bases $\{|x_0\rangle, |x_1\rangle, \ldots, |x_{n-1}\rangle\}$ and $\{|y_0\rangle, |y_1\rangle, \ldots, |y_{m-1}\rangle\}$, respectively, then an arbitrary vector in $V \otimes W$ is a linear combination of the *nm* basis vectors $|x_i\rangle \otimes |y_j\rangle = |x_i y_j\rangle$.

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |x_i y_j\rangle \in V \otimes W$$

$$|\psi\rangle = \sum_{i,j} \psi_{ij} |x_i y_j\rangle \in V \otimes W$$

Notice these coefficients can assemble into an n×m matrix...

$$\begin{array}{c c} & \begin{array}{cc} j=0 & j=1 \end{array} \\ \begin{array}{c} i=0 \\ i=1 \\ i=2 \end{array} & \begin{bmatrix} \psi_{00} & \psi_{01} \\ \psi_{10} & \psi_{11} \\ \psi_{20} & \psi_{21} \end{bmatrix} \end{array}$$

So, actually...

Technically speaking, the tensor product of coordinate vectors in $V \otimes W$ is called their **outer product,** which is a matrix representing a linear transformation from W to V.

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Technically speaking, the tensor product of coordinate vectors in $V \otimes W$ is called their **outer product,** which is a matrix representing a linear transformation from W to V.

$$|vw\rangle \leftrightarrow |v\rangle\langle w| = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \begin{bmatrix} 4 & 5 \end{bmatrix} = \begin{bmatrix} 1\cdot 4 & 1\cdot 5 \\ 2\cdot 4 & 2\cdot 5 \\ 3\cdot 4 & 3\cdot 5 \end{bmatrix} = \begin{bmatrix} 4 & 5 \\ 8 & 10 \\ 12 & 15 \end{bmatrix}$$

(The one-to-one correspondence between bras $\langle w|$ and kets $|w\rangle$ gives the change in perspective between 1D arrays and matrices.)

More formally, this correspondence is the statement that the tensor product $V \otimes W$ is isomorphic to the space of linear maps $W^* \to V$, where W^* is called the *dual space* associated to W, whose bases are the bras $\langle i|$.

Quick facts

scalar multiplication

$$k(|v\rangle \otimes |w\rangle) = k|v\rangle \otimes |w\rangle = |v\rangle \otimes k|w\rangle$$

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Tensor product distributes over addition

$$\left(|u\rangle + |v\rangle\right) \otimes |w\rangle = |u\rangle \otimes |w\rangle + |v\rangle \otimes |w\rangle$$

$$|u\rangle \otimes \left(|v\rangle + |w\rangle\right) = |u\rangle \otimes |v\rangle + |u\rangle \otimes |w\rangle$$

Quick facts

scalar multiplication

$$k\left(|v\rangle \otimes |w\rangle\right) = k|v\rangle \otimes |w\rangle = |v\rangle \otimes k|w\rangle$$

Tensor product distributes over addition

$$\left(|u\rangle + |v\rangle\right) \otimes |w\rangle = |u\rangle \otimes |w\rangle + |v\rangle \otimes |w\rangle$$

$$|u\rangle \otimes \left(|v\rangle + |w\rangle\right) = |u\rangle \otimes |v\rangle + |u\rangle \otimes |w\rangle$$

associativity

$$\left(|u\rangle \otimes |v\rangle\right) \otimes |w\rangle = |u\rangle \otimes \left(|v\rangle \otimes |w\rangle\right)$$

Tensor product vs. direct sum

Besides the tensor product, there's another way to combine two vector spaces: the **direct sum** (or *Cartesian product*).

$$\mathbb{C}^n \oplus \mathbb{C}^m \quad \ldots \quad \dim(\mathbb{C}^n \oplus \mathbb{C}^m) = n + m$$

We won't go into detail – *and it's not used to model composite quantum systems* – but it's good to be aware of. Here's an easy way to think about it....

tensor product

$$|vw\rangle = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \otimes \begin{bmatrix} 4 \\ 5 \end{bmatrix} = \begin{bmatrix} 4 \\ 5 \\ 8 \\ 10 \\ 12 \\ 15 \end{bmatrix}$$

$$\mathbb{R}^3 \otimes \mathbb{R}^2 \cong \mathbb{R}^{3\times 2}$$

dimensions **multiply**

direct sum

$$|v,w\rangle = \left(\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \begin{bmatrix} 4 \\ 5 \end{bmatrix} \right) \rightsquigarrow \begin{bmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{bmatrix}$$

$$\mathbb{R}^3 \oplus \mathbb{R}^2 \cong \mathbb{R}^{3+2}$$

dimensions **add**

Exercises

$\boxed{1}$ Find the array representations of the eight basis vectors of $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, where $\mathbb{C}^2$ has bases $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

$|000\rangle = ?$ $\quad |100\rangle = ?$ $\quad |010\rangle = ?$ $\quad |001\rangle = ?$ $\quad$ etc.

$\boxed{2}^*$ Let $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \in \mathbb{C}^2$. Write out $|\psi\rangle \otimes |\psi\rangle$ explicitly.

$\boxed{3}$ Prove that $\langle vw | ab \rangle = \langle v | a \rangle \langle w | b \rangle$ for all vectors $|v\rangle, |a\rangle \in \mathbb{C}^n$ and $|w\rangle, |b\rangle \in \mathbb{C}^m$.

$\boxed{4}$ Prove that $|\psi\rangle \otimes |\phi\rangle$ is a unit vector whenever both $|\psi\rangle$ and $|\phi\rangle$ are unit vectors. (<u>Hint</u>: use $\boxed{3}$.)

Break

(5 min.)

Solution Walk-Through

(5 min.)

Solution #2

$$|\psi\rangle \otimes |\psi\rangle =$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Solution #2

$$|\psi\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Solution #2

$$|\psi\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

move scalar
out front

$$= \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \left(|0\rangle + |1\rangle\right)$$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Solution #2

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|\psi\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

move scalar out front

$$= \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \left(|0\rangle + |1\rangle\right)$$

distribute $\otimes$

$$= \frac{1}{2}\left(|0\rangle \otimes \left(|0\rangle + |1\rangle\right) + |1\rangle \otimes \left(|0\rangle + |1\rangle\right)\right)$$

Solution #2

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$|\psi\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

move scalar out front

$$= \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \otimes \left(|0\rangle + |1\rangle\right)$$

distribute $\otimes$

$$= \frac{1}{2}\left(|0\rangle \otimes \left(|0\rangle + |1\rangle\right) + |1\rangle \otimes \left(|0\rangle + |1\rangle\right)\right)$$

distribute $\otimes$ again!

$$= \frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle + |11\rangle\right)$$

Solution #2

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

Alternatively,

$$|\psi\rangle \otimes |\psi\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \otimes \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1\\1\end{bmatrix} \otimes \begin{bmatrix}1\\1\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix}$$

$$= \frac{1}{2}\left(\underbrace{\begin{bmatrix}1\\0\\0\\0\end{bmatrix}}_{|00\rangle} + \underbrace{\begin{bmatrix}0\\1\\0\\0\end{bmatrix}}_{|01\rangle} + \underbrace{\begin{bmatrix}0\\0\\1\\0\end{bmatrix}}_{|10\rangle} + \underbrace{\begin{bmatrix}0\\0\\0\\1\end{bmatrix}}_{|11\rangle}\right)$$

$$= \frac{1}{2}\left(|00\rangle + |01\rangle + |10\rangle + |11\rangle\right)$$

Break

(10 min.)

Tensor Products, cont.

How can we understand *linear transformations* between tensor products of vector spaces?

$$\mathbb{C}^n \xrightarrow{M} \mathbb{C}^a$$

$$\mathbb{C}^m \xrightarrow[N]{} \mathbb{C}^b$$

$$\begin{tikzcd}
\mathbb{C}^n \arrow[r, "M"] & \mathbb{C}^a \\
\mathbb{C}^m \arrow[r, "N"'] & \mathbb{C}^b
\end{tikzcd}$$

$$\begin{tikzcd}
\otimes & \otimes
\end{tikzcd}$$

$$\begin{array}{ccc} \mathbb{C}^n & & \mathbb{C}^a \\ \otimes & \longrightarrow & \otimes \\ \mathbb{C}^m & & \mathbb{C}^b \end{array}$$

familiar thing

familiar thing

$$\mathbb{C}^n \otimes \mathbb{C}^m \xrightarrow{M \otimes N} \mathbb{C}^a \otimes \mathbb{C}^b$$

What’s this?

Linear transformations of the form $M \otimes N$ are easy to understand. If $|v\rangle$ is a vector in $\mathbb{C}^n$ and $|w\rangle$ is a vector in $\mathbb{C}^m$, then we define

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So in general, if $|\psi\rangle$ is an arbitrary vector in $\mathbb{C}^n \otimes \mathbb{C}^m$, then

$$|\psi\rangle = \sum \psi_{ij} |ij\rangle \quad \Rightarrow$$

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$$|\psi\rangle = \sum \psi_{ij} |ij\rangle \quad \Rightarrow \quad (M \otimes N)|\psi\rangle = \sum_{ij} \psi_{ij} M|i\rangle \otimes N|j\rangle$$

Matrix Representations

Suppose we've chosen bases for our vector spaces, so that we may consider the *matrix representations* of the linear maps M and N.

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Suppose we've chosen bases for our vector spaces, so that we may consider the *matrix representations* of the linear maps M and N.

The matrix representation of the linear map $M \otimes N$ is obtained by the **Kronecker product** of the respective matrices.

$$\mathbb{C}^n \otimes \mathbb{C}^m \xrightarrow{M \otimes N} \mathbb{C}^a \otimes \mathbb{C}^b$$

More generally, an arbitrary linear map from is a linear combination of maps of the form $|i'\rangle\langle i| \otimes |j'\rangle\langle j|$ where $\{|ij\rangle\}$ is a basis for $\mathbb{C}^n \otimes \mathbb{C}^m$ and where $\{|i'j'\rangle\}$ is a basis for $\mathbb{C}^a \otimes \mathbb{C}^b$.

$$M = \begin{bmatrix} 1 & 2 \\ -3 & 0 \end{bmatrix}$$

$$M \otimes N =$$

$$N = \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix}$$

$$M = \begin{bmatrix} 1 & 2 \\ -3 & 0 \end{bmatrix}$$

$$N = \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix}$$

$$M \otimes N = \begin{bmatrix} 1 \cdot N & 2 \cdot N \\ -3 \cdot N & 0 \cdot N \end{bmatrix}$$

$$M = \begin{bmatrix} 1 & 2 \\ -3 & 0 \end{bmatrix}$$

$$N = \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix}$$

$$M \otimes N = \begin{bmatrix} 1 \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix} & 2 \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix} \\ -3 \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix} & 0 \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix} \end{bmatrix}$$

$$M = \begin{bmatrix} 1 & 2 \\ -3 & 0 \end{bmatrix}$$

$$N = \begin{bmatrix} 0 & 2 \\ -1 & 4 \\ 5 & 0 \end{bmatrix}$$

$$M \otimes N = \begin{bmatrix} 0 & 2 & 0 & 4 \\ -1 & 4 & -2 & 8 \\ 5 & 0 & 10 & 0 \\ 0 & -6 & 0 & 0 \\ 3 & -12 & 0 & 0 \\ -15 & 0 & 0 & 0 \end{bmatrix}$$

Quick facts

$$(M \otimes N)(M' \otimes N') = MM' \otimes NN'$$

"The composition of tensor products is the tensor product of the compositions."

Exercise:
verify these equalities!

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"Complex conjugation distributes over the tensor product."

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$$(M \otimes N)^T = M^T \otimes N^T$$

"Transposition distributes over the tensor product."

$$(M \otimes N)^\dagger = M^\dagger \otimes N^\dagger$$

"The conjugate transpose distributes over the tensor product."

Exercise:
verify these equalities!

Graphical Notation

There is a convenient graphical notation for linear maps and their tensor products called **tensor network diagram notation**. Here’s a brief introduction.

Terminology

Let's refer to an n-dimensional array of numbers as a **tensor of order n**, or more simply an **n-tensor**.

- 0 tensor = number
- 1 tensor = vector
- 2 tensor = matrix
- 3-tensor = 3-tensor
- ...

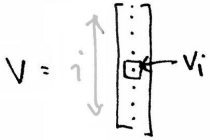
We can visually represent an n-tensor as a *node* with n *edges*.

a number

a number

a vector

v_i



a number

a vector

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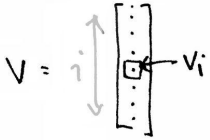
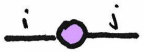
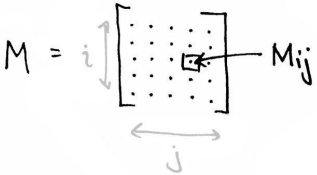


a matrix



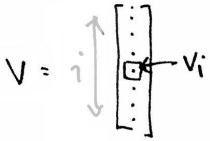
M_{ij}



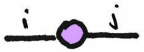
a number

a vector

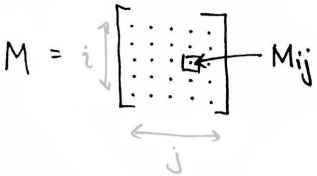
v_i



a matrix

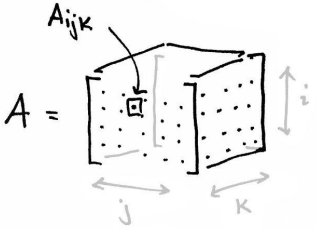


M_{ij}



a 3-tensor

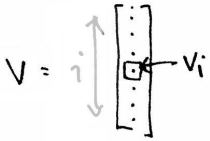
A_{ijk}



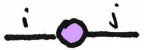
a number

a vector

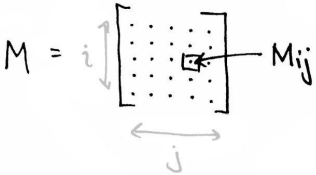
v_i



a matrix

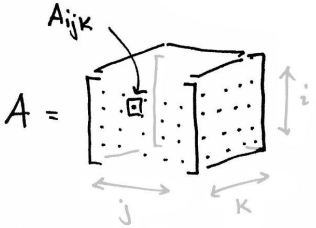


M_{ij}

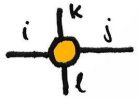


a 3-tensor

A_{ijk}



a 4-tensor



B_{ijkl}

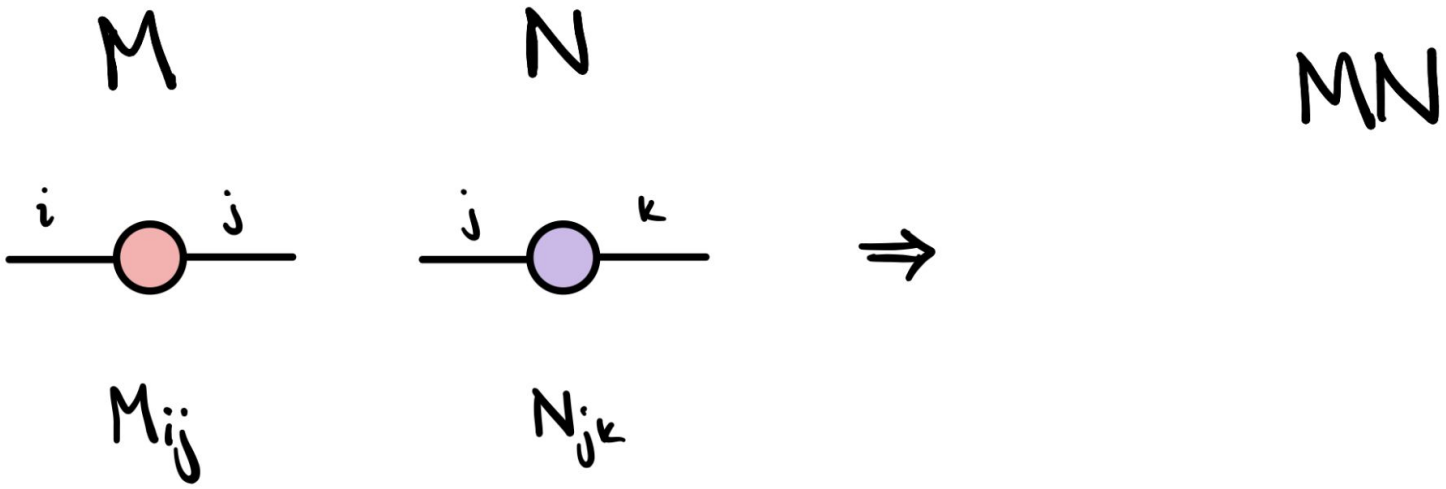
B = (4-dimensional cube ...)

⋮ ⋮ ⋮ ⋮

Bonus: Familiar operations have nice pictures!

---------- →

Matrix multiplication corresponds to joining edges.



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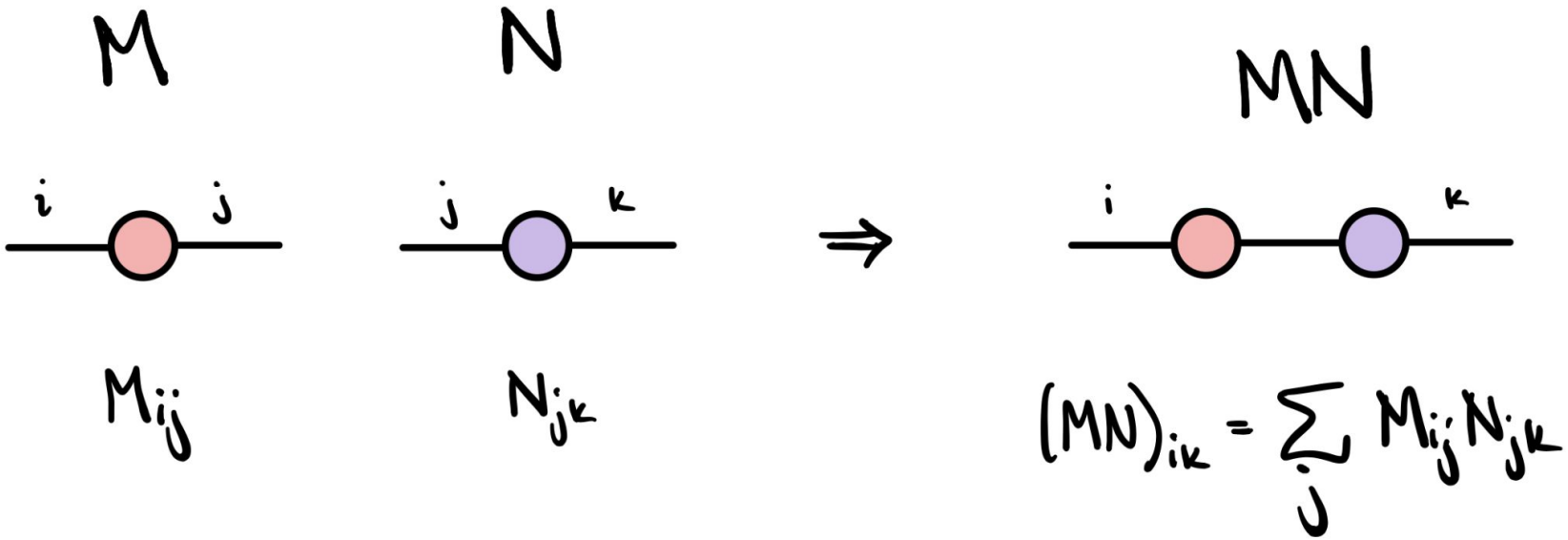

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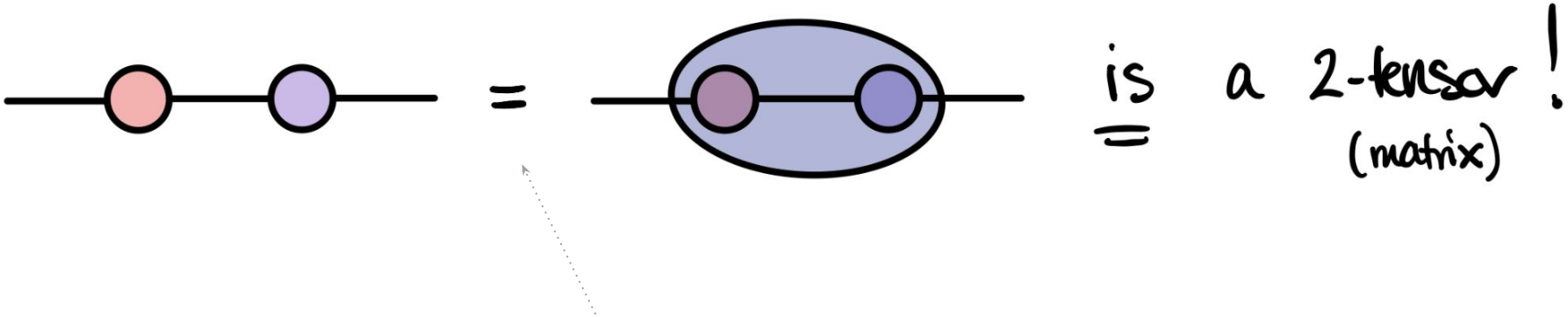
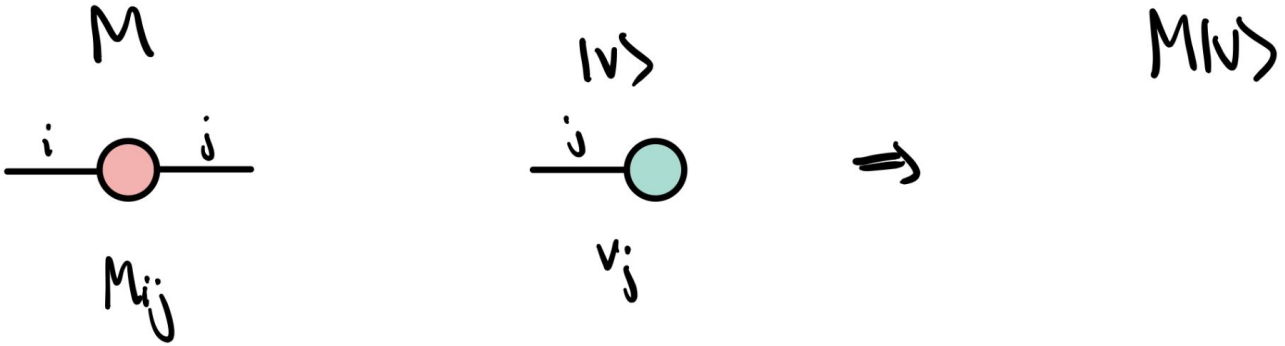
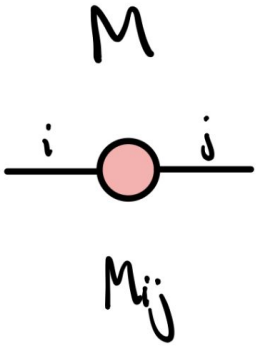


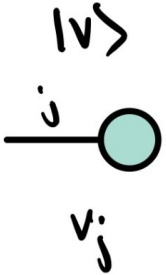
Imagine smushing the nodes together.

Matrix-vector multiplication corresponds to joining edges.

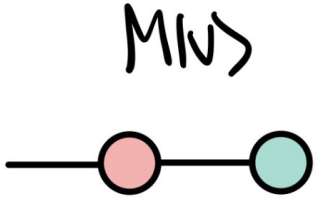


Matrix-vector multiplication corresponds to joining edges.

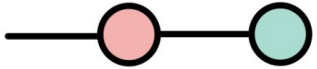




$\Rightarrow$

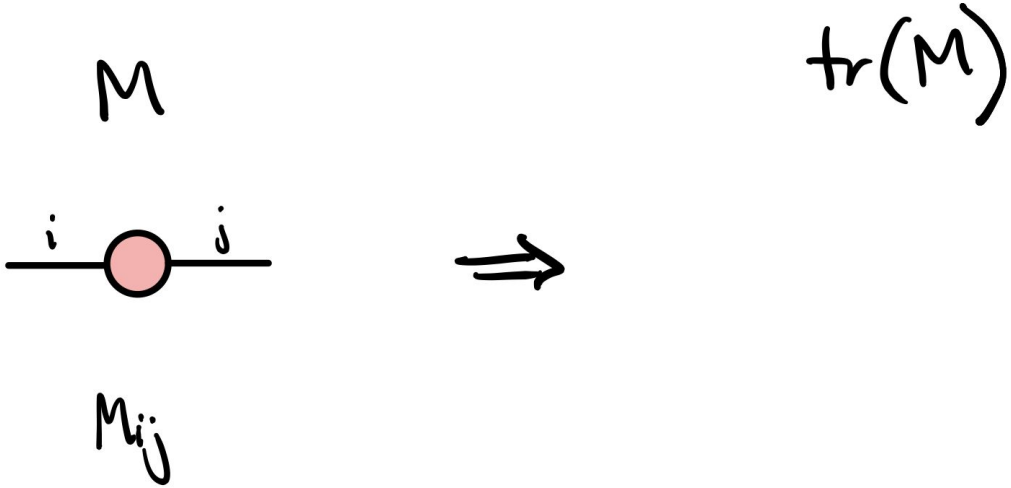


$$(M|v\rangle)_i = \sum_j M_{ij} v_j$$



is a 1-tensor! (vector)

The trace of a matrix is a node with a loop.



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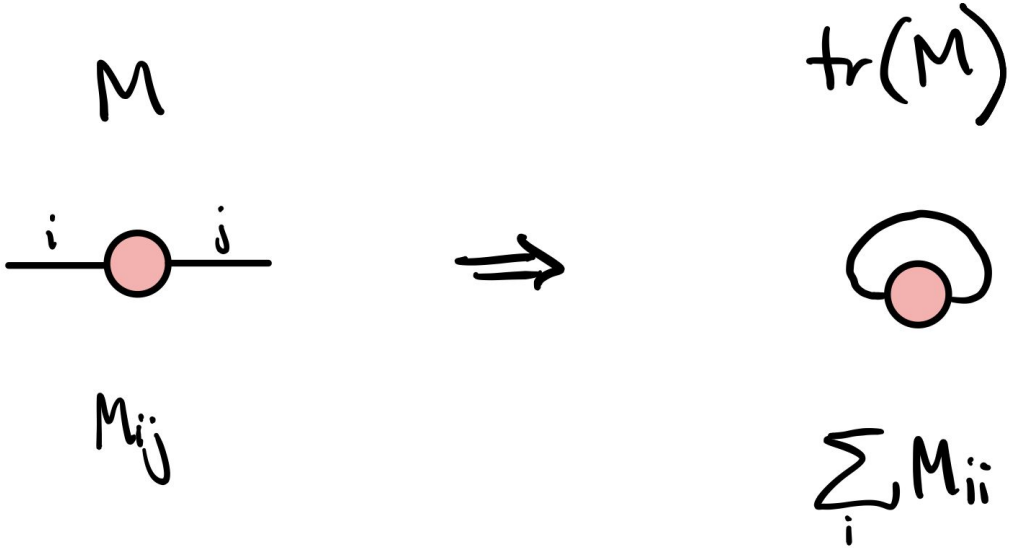
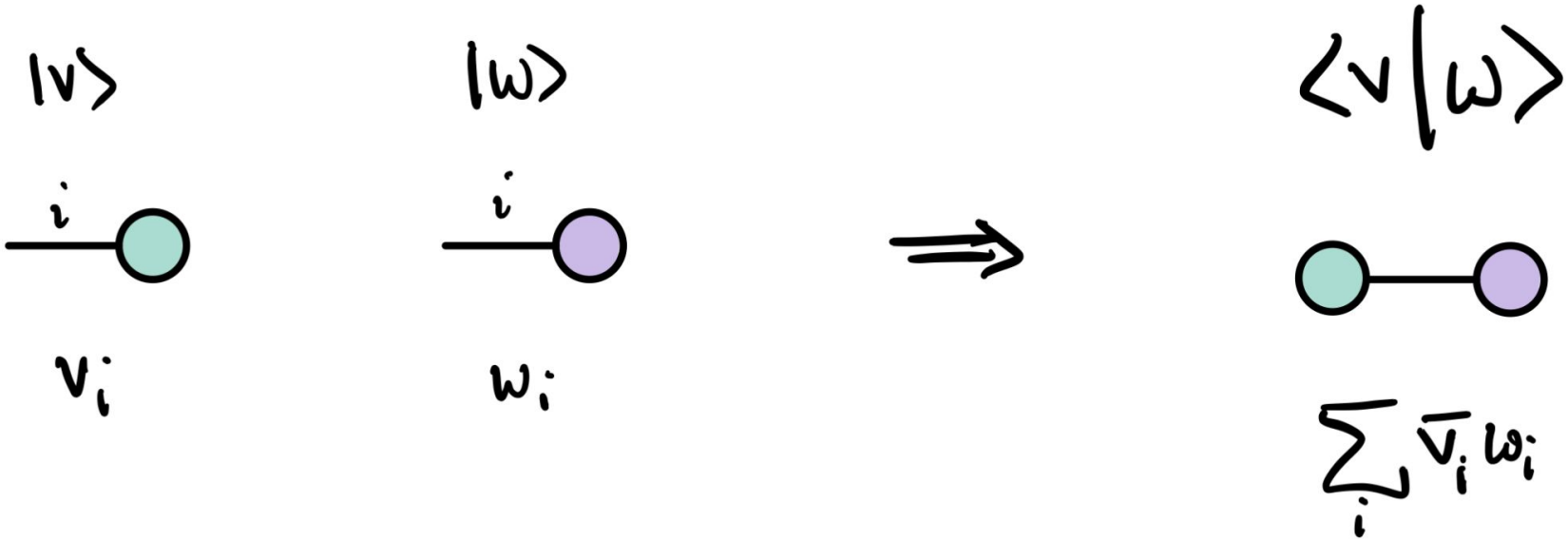
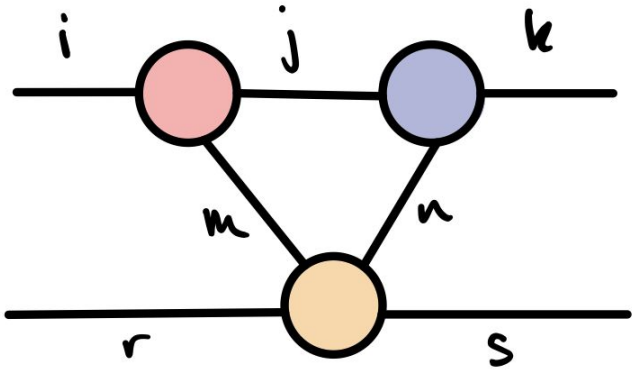


The inner product of vectors is a dumbbell.

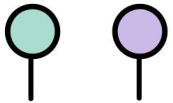


More generally, summing along a common index, i.e. “tensor contraction,” is visualized by joining the corresponding edges.

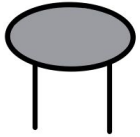


$$= \sum_{j,m,n} A_{ijm} B_{jnk} C_{rmns}$$

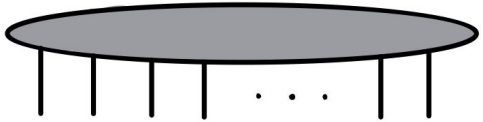
Tensor products are visualized by stacking side-by-side.



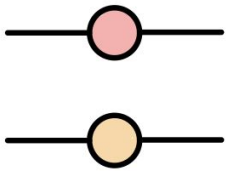
$$|v\rangle \otimes |w\rangle$$



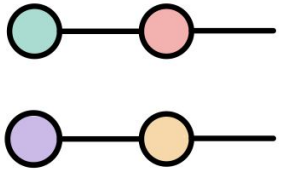
$$|\psi\rangle = \sum_{i,j} \psi_{ij} |i\rangle \otimes |j\rangle$$



$$= \sum_{i_1, i_2, \ldots, i_N} T_{i_1 i_2 \cdots i_N} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle$$

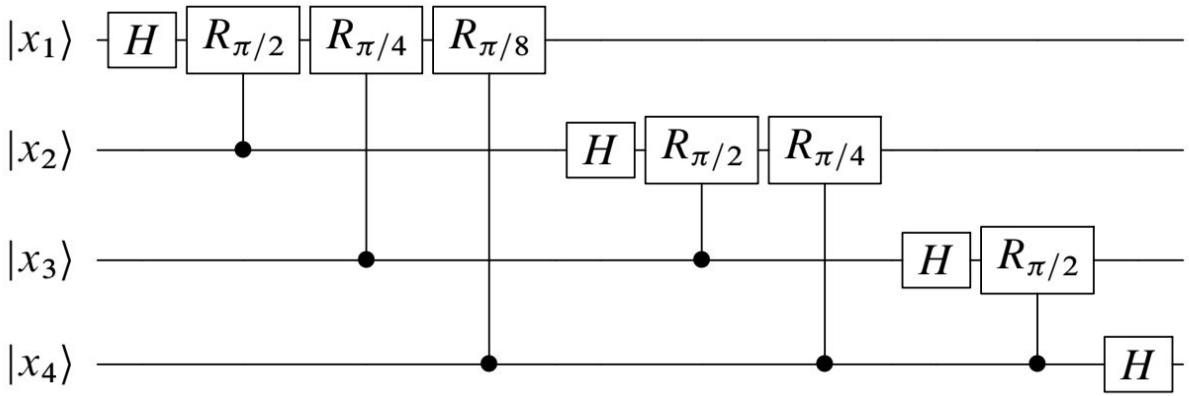


$$M \otimes N$$



$$(M \otimes N)(|v\rangle \otimes |w\rangle) = M|v\rangle \otimes N|w\rangle$$

This notation is closely related to **quantum circuit diagrams**, to be covered in future sessions.



A quantum circuit diagram corresponding to a quantum Fourier transform. Image from *Quantum Computing: An Applied Approach* by Jack Hidary.

Exercises

1. Prove that the composition of two Hermitian operators is Hermitian, then prove that the tensor product of two Hermitian operators is Hermitian.

2.* Prove that the composition of two unitary operators is unitary, then prove that the tensor product of two unitary operators is unitary.

3. Let $CNOT = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$ represent a linear operator on $\mathbb{C}^2 \otimes \mathbb{C}^2$. Compute $CNOT|ij\rangle$ for each $i=0,1$ and $j=0,1$.

4. Let $H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ represent a linear operator on $\mathbb{C}^2$. Compute the vector $\left(CNOT \circ (H \otimes I)\right)|00\rangle$, where $I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ is the identity matrix and the composition symbol $\circ$ is matrix multiplication.

Break

(5 min.)

Solution Walk-Through

(5 min.)

Solution #2.

Suppose U and V are unitary operators on $\mathbb{C}^n$.

$$UU^\dagger = U^\dagger U = I \qquad VV^\dagger = V^\dagger V = I.$$

<u>fact</u>: $(AB)^\dagger = B^\dagger A^\dagger$

Solution #2.

(composition) "UV is unitary" means

This is what we want to show.

$$(UV)^{+}(UV) = (UV)(UV)^{+} = I.$$

Solution #2.

(composition) "UV is unitary" means

This is what we want to show.

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Conjugate transpose distributes over $\otimes$ (see prev. slides)

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The composition of tensor products is the tensor product of compositions. (see prev. slides)

$$= U^\dagger U \otimes V^\dagger V$$

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The composition of tensor products is the tensor product of compositions. (see prev. slides)

$$= U^\dagger U \otimes V^\dagger V$$

U and V are both unitary

$$= I \otimes I$$

$$= I$$

(and similarly).

Today's Agenda

- Eigenvectors / Eigenvalues
  - Motivation
  - Definition and examples
- Spectral Theorem
  - Spectral decomposition
- Singular Value Decomposition
  - Entanglement

Eigenvectors / Eigenvalues

Motivation: To understand the behavior of a linear operator, it's often helpful to look at subspaces that are "fixed" by it.

These are called *invariant subspaces*.

Idea: Understand a linear operator by studying smaller “pieces” of it.

Example:

A vector space of polynomials.

Consider the set P_5 of polynomials of degree at most 5 with real coefficients.

$$p(x) = 3 + 2x^2 - x^5$$

$$q(x) = x - 7x^4$$

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This is a vector space.

$$p(x) + q(x) \in P_5 \quad \checkmark$$

Closed under addition.

a real number

$$k\,p(x) \in P_5 \quad \checkmark$$

Closed under scalar multiplication.

Example: Differentiation is a linear operator.

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Consider the function M: $P_5 \to P_5$ defined by differentiation, $M(p(x)) = p'(x)$.

$$M(p(x)) = M(3 + 2x^2 - x^5) = 4x - 5x^4 = p'(x)$$

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This is a linear operator.

$$M(p(x) + q(x)) = p'(x) + q'(x) = M(p(x)) + M(q(x))$$

Follows from calculus: the derivative of the sum is the sum of the derivatives.

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Consider the function $M: P_5 \to P_5$ defined by differentiation, $M(p(x)) = p'(x)$.

$$M(p(x)) = M(3 + 2x^2 - x^5) = 4x - 5x^4 = p'(x)$$

This is a linear operator.

the chain rule

$$M(kp(x)) = \cancel{k'p(x)} + kp'(x) = kM(p(x))$$

The derivative of a constant is 0.

Observation

Consider the subspace $P_3 \subseteq P_5$ consisting of polynomials of degree at most 3. It is **invariant** under the linear operator M.

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Consider the subspace $P_3 \subseteq P_5$ consisting of polynomials of degree at most 3. It is **invariant** under the linear operator M.

If $p(x) \in P_3$ then $M(p(x)) \in P_3$, too.

"If the degree of p(x) is at most 3.."

"...then the degree of its derivative p'(x) is at most 3, too."

Given a linear operator $M: V \to V$,

a subspace $\mathcal{U} \subseteq V$ is called <u>invariant</u>

<u>under M</u> if "$|u\rangle \in \mathcal{U}$" implies "$M|u\rangle \in \mathcal{U}$".

"Whatever's in U *stays* in U."

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Example

P_3 is a **4-dimensional invariant subspace** of the differentiation operator $M: P_5 \to P_5$.

That’s nice. Here’s something easier:

1-dimensional invariant subspaces

One-dimensional subspaces of a vector space V are easy to understand.

Pick any vector $|v\rangle$ in V and consider all scalar multiples of it. This is a 1-dimensional subspace of V.

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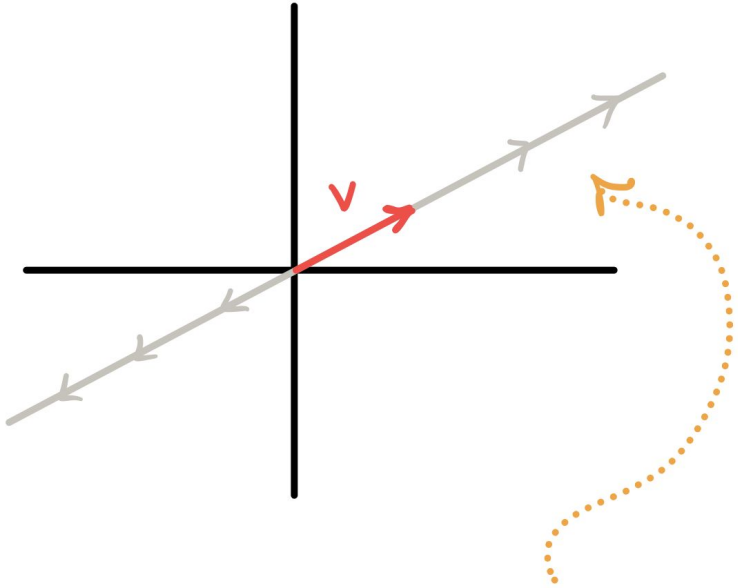
$$\mathcal{U} = \{\lambda|v\rangle : \lambda \in \mathbb{C} \text{ or } \mathbb{R}\}$$



This line is the set

$$\{\lambda|v\rangle : \lambda \in \mathbb{C} \text{ or } \mathbb{R}\}$$

Now consider a linear operator M: V → V. *What does it mean for the 1-dimensional subspace U to be* ***invariant under M****?* Recall the definition:

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$\mathcal{U} = \{\lambda|v\rangle : \lambda \text{ is a number}\}$ is invariant under M if

"$|v\rangle \in \mathcal{U}$" implies "$M|v\rangle \in \mathcal{U}$".

Now consider a linear operator M: V → V. *What does it mean for the 1-dimensional subspace U to be* ***invariant under M****?* Recall the definition:

$\mathcal{U} = \{\lambda|v\rangle : \lambda \text{ is a number}\}$ is invariant under M if

"$|v\rangle \in \mathcal{U}$" implies $\boxed{\text{"}M|v\rangle \in \mathcal{U}\text{".}}$

This means
$M|v\rangle = \lambda|v\rangle$
for some scalar λ.

A scalar λ is called an **eigenvalue** of a linear operator $M: V \to V$ if there is a *nonzero* vector $|v\rangle$ in V so that

"eigenvalue"

$$\boxed{M|v\rangle = \lambda|v\rangle}$$

"eigenvector"

in which case $|v\rangle$ is called the **eigenvector** of M corresponding to the eigenvalue λ.

We exclude the possibility that $|v\rangle = 0$ (the vector of all zeros), since otherwise $M0 = \lambda 0$ would be true for every operator M and every scalar λ, which isn't interesting.

Two perspectives:

Geometric vs. Algebraic

Geometric Perspective

As an example, consider a 2×2 matrix.

Consider the following 2×2 matrix, which represents a linear operator M: $\mathbb{R}^2 \to \mathbb{R}^2$. Does it have an eigenvector?

$$M = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$$

To find out, let's see the transformation M "in action."

See "Eigenvectors and Eigenvalues" at 2:39 by Grant Sanderson (3Blue1Brown).

If $M = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$ then $|v\rangle = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$

is an eigenvector with

eigenvalue $\lambda = 2$:

$$M|v\rangle = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} -1 \\ 1 \end{bmatrix} = \begin{bmatrix} -2 \\ 2 \end{bmatrix} = 2\begin{bmatrix} -1 \\ 1 \end{bmatrix} = \lambda|v\rangle$$

Algebraic Perspective

How to find eigenvalues/vectors?

$$M|v\rangle = \lambda|v\rangle$$

$$M|v\rangle = \lambda|v\rangle \quad \overset{\text{“if and only if”}}{\Longleftrightarrow} \quad M|v\rangle - \lambda|v\rangle = 0$$

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$$\Longleftrightarrow \quad (M - \lambda I)|v\rangle = 0$$

$$\lambda I = \lambda \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix}$$

$$= \begin{bmatrix} \lambda & & & \\ & \lambda & & \\ & & \ddots & \\ & & & \lambda \end{bmatrix}$$

I is notation for the n×n identity matrix.

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$$\Longleftrightarrow \quad M - \lambda I \text{ is not injective}$$

A linear map is “injective” iff the only vector it sends to 0 is the zero vector.

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$$\Longleftrightarrow \quad \det(M - \lambda I) = 0$$

“Determinant”?

Given any square matrix M, we can obtain a number from its entries called the **determinant of M.**

$\det M = 0$ iff

M is <u>not</u> invertible.

$$\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$$

Characteristic equation

An n×n matrix M has an eigenvalue λ if and only if

$$\det(M - \lambda I) = 0$$

Characteristic equation

An n×n matrix M has an eigenvalue λ if and only if

$$\underbrace{\det(M - \lambda I)}_{\text{"characteristic polynomial of M"}} = 0$$

Example

$\boxed{\text{Example}}$ Suppose $M = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}$. consider the matrix $M - \lambda I$.

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iff $\boxed{\lambda = 3,\ \lambda = 2}$ ← eigenvalues of M

$\boxed{\text{Example}}$ How to find the eigen<u>vector</u> corresponding to $\lambda = 2$?

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$$(M - \lambda I)|v\rangle = 0 \xrightarrow{\text{"plug and chug"}} \left(\begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} - \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \right) \underbrace{\begin{bmatrix} x \\ y \end{bmatrix}}_{\text{let } v = \begin{bmatrix} x \\ y \end{bmatrix}} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

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$$\Leftrightarrow |v\rangle = \begin{bmatrix} -y \\ y \end{bmatrix} \longrightarrow \boxed{|v\rangle = \begin{bmatrix} -1 \\ 1 \end{bmatrix}}$$

“Eigenvectors and Eigenvalues” at 2:39 by Grant Sanderson (3Blue1Brown).

Break

(5 min.)

Spectral Theorem

Does every matrix always have eigenvalues and eigenvectors? The answer is certainly “no” for *rectangular* matrices. How about all square matrices?

Do all square matrices have eigenvalues?

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NO. As an example, consider the matrix representing CCW rotation by 90° in $\mathbb{R}^2$.

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$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$$

Check:

The characteristic polynomial of this matrix is $p(\lambda)=\lambda^2+1$ which does not have solutions in $\mathbb{R}$. *No coincidence.*

Are *any* matrices guaranteed to have eigenvalues / eigenvectors? Yes...

Spectral Theorem

Let M be a **Hermitian** operator on the complex vector space $\mathbb{C}^n$ of dimension n. Then M has an *orthonormal* set of n eigenvectors $\{|u_1\rangle, |u_2\rangle, ..., |u_n\rangle\}$ with eigenvalues $\{\lambda_1, \lambda_2, ..., \lambda_n\}$.

Moreover,

Spectral Theorem

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Moreover,

$$M = \lambda_1 |u_1\rangle\langle u_1| + \lambda_2 |u_2\rangle\langle u_2| + \cdots + \lambda_n |u_n\rangle\langle u_n|$$

Recall, each $|u_i\rangle\langle u_i|$ is the outer product of the ith eigenvector of M with itself. In other words, $|u_i\rangle\langle u_i|$ is the rank 1 projection operator onto the line spanned by $|u_i\rangle$.

Spectral Decomposition

$$\boxed{M = \lambda_1 |u_1\rangle\langle u_1| + \lambda_2 |u_2\rangle\langle u_2| + \cdots + \lambda_n |u_n\rangle\langle u_n|}$$

the **spectral decomposition** of M

*Why? The set of eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ is called the **spectrum** of M.*

More succinctly...

There exist a **unitary operator** U and a **diagonal operator** D so that

$$M = UDU^{-1}$$

$$U = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_n \\ | & | & & | \end{bmatrix}$$

The columns of U
are the **eigenvectors** of M.

$$D = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

The diagonal entries of D
are the **eigenvalues** of M.

Proof of Spectral Theorem

Omit.

The theorem holds more generally for **normal operators**, of which self-adjoint (i.e. Hermitian) operators are an example.

See Axler's *Linear Algebra Done Right*.

Example

$\boxed{\text{Example}}$

The matrix $M = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}$ has eigenvectors/values:

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$$\begin{cases} \lambda_0 = 3 \\ |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \end{cases} \quad \& \quad \begin{cases} \lambda_1 = 2 \\ |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{cases}$$

By the Spectral Theorem, M can be written as

$$M = 3|0\rangle\langle 0| + 2|1\rangle\langle 1|$$

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$$= 3\begin{bmatrix}1 & 0\\0 & 0\end{bmatrix} + 2\begin{bmatrix}0 & 0\\0 & 1\end{bmatrix}$$

$$= \begin{bmatrix}3 & 0\\0 & 2\end{bmatrix} \checkmark$$

or more succinctly ...

first column is $|0\rangle$

second column is $|1\rangle$

Diagonals are eigenvalues

$$M = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= U \quad D \quad U^{-1}$$

or more succinctly ...

first column is $|0\rangle$

second column is $|1\rangle$

Diagonals are eigenvalues

BORING.

$$= U D U^{-1}$$

more interesting

$\boxed{\text{Example}}$

more interesting

Example

The matrix $M = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ has

three eigenvalues & eigenvectors:

more interesting

Example

The matrix $M = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$ has

three eigenvalues & eigenvectors:

$$\lambda_1 = 2, \ |u_1\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix} \qquad \lambda_2 = 1, \ |u_2\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \qquad \lambda_3 = 0, \ |u_3\rangle = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}$$

By the Spectral Theorem, M may be written as

$$M = \lambda_1 |u_1\rangle\langle u_1| + \lambda_2 |u_2\rangle\langle u_2| + \lambda_3 |u_3\rangle\langle u_3|$$

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$$M = \lambda_1 |u_1\rangle\langle u_1| + \lambda_2 |u_2\rangle\langle u_2| + \lambda_3 |u_3\rangle\langle u_3|$$

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

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

$$= \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \checkmark$$

or more succinctly ...

$$M = \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}}_{U^{-1}}$$

or more succinctly ...

first column is $|u_1\rangle$

second column is $|u_1\rangle$

third column is $|u_3\rangle$

diagonals are eigenvalues

$$M = \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{D} \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}}_{U^{-1}}$$

$$\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = U \begin{bmatrix} 2 & & \\ & 1 & \\ & & 0 \end{bmatrix} U^{-1}$$

$$\underbrace{\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{not diagonal } \times} = U \underbrace{\begin{bmatrix} 2 & & \\ & 1 & \\ & & 0 \end{bmatrix}}_{\text{diagonal } \checkmark} U^{-1}$$

implies

$$\underbrace{\begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{not diagonal } \times} = U \underbrace{\begin{bmatrix} 2 & & \\ & 1 & \\ & & 0 \end{bmatrix}}_{\text{diagonal } \checkmark} U^{-1}$$

implies

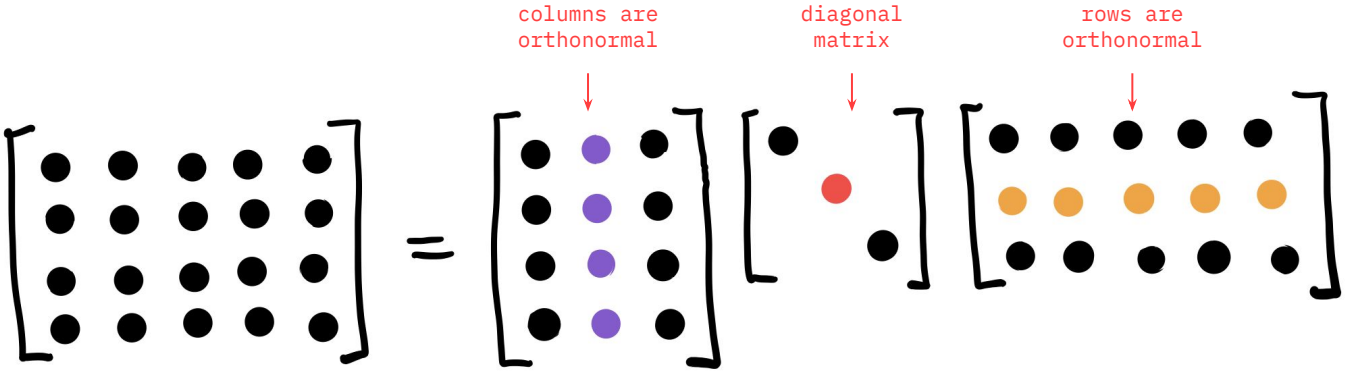
"M is diagonal
(i.e. easy to work with)
up to a change in perspective."

$$U^{-1} M U = \underbrace{\begin{bmatrix} 2 & & \\ & 1 & \\ & & 0 \end{bmatrix}}_{\text{diagonal } \checkmark}$$

The Spectral Theorem is powerful. But what about matrices that aren’t square?

Singular Value Decomposition

Theorem: Every n×m matrix M can be written as



$$M = U D V^{\dagger}$$

M: $n \times m$ $\quad U$: $n \times k$ $\quad D$: $k \times k$ $\quad V^{\dagger}$: $k \times m$

$k = \text{rank}(M)$

Singular Value Decomposition

Theorem: Every $n \times m$ matrix M can be written as

"Every"!

Don't think of SVD as a second-rate theorem.

It's a powerful statement.

In general, factorization is **hard**. Modern cryptography is based on this fact.

And yet in linear algebra, **every** matrix — not just those with special properties — can be factored in this very nice way.

Singular Value Decomposition

Theorem: Every n×m matrix M can be written as

$$M = UDV^T$$

Columns of U are called the **left singular vectors** of M.

Entries along the diagonal of D are called the **singular values** of M.

Columns of V are called the **right singular vectors** of M.

Okay. So what?

Many answers. Here’s one.

So what?

Consider an arbitrary unit vector in a tensor product space.

$$|\psi\rangle = \sum_{ij} \psi_{ij} |ij\rangle \in \mathbb{C}^n \otimes \mathbb{C}^m$$

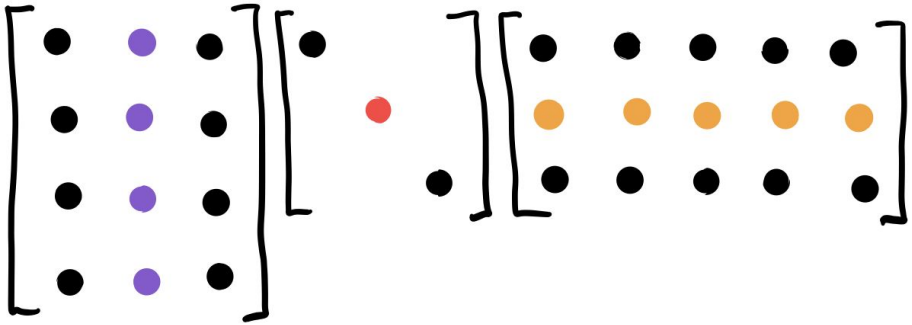
$|\psi\rangle$ may represent the state of some composite, 2-object system.

Recall that the coefficients ψ_{ij} assemble into an n×m matrix....

$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \vdots & \\ \cdots & \psi_{ij} & \\ & & \end{bmatrix} \end{array}$$

$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \psi_{ij} & \end{bmatrix} \end{array}$$

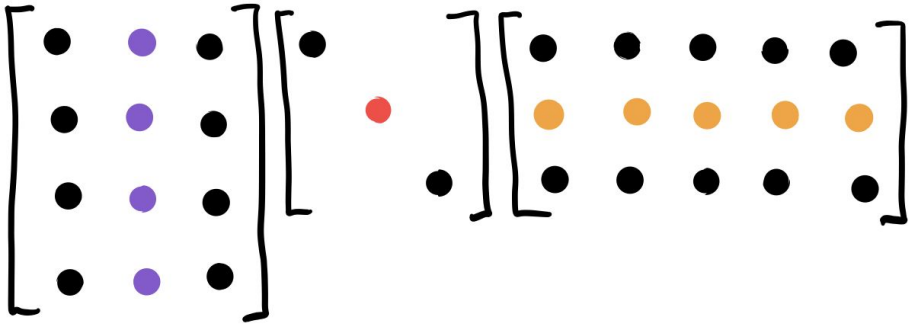
$$\overset{\text{SVD}}{=}$$



$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \psi_{ij} & \end{bmatrix} \end{array}$$

The number of non-zero singular values is called the **Schmidt rank** of the quantum state $|\psi\rangle$. It is a measure of entanglement between the two subsystems.

$$\overset{\text{SVD}}{=}$$

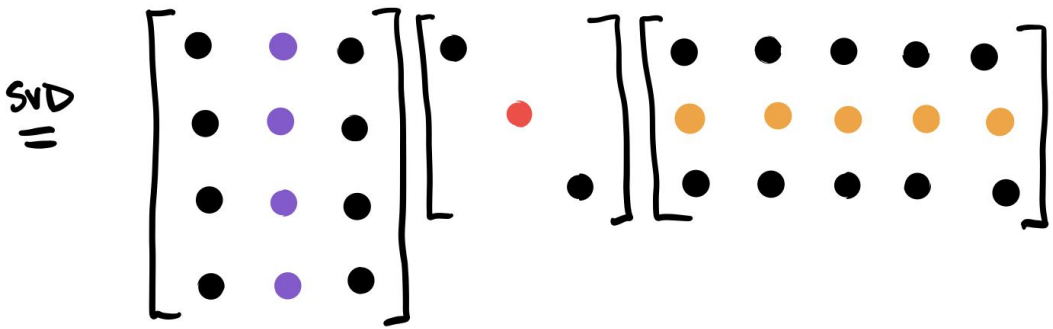


$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \vdots & \\ \cdots & \psi_{ij} & \\ & & \end{bmatrix} \end{array}$$

The number of non-zero singular values is called the **Schmidt rank** of the quantum state $|\psi\rangle$. It is a measure of entanglement between the two subsystems.

The state $|\psi\rangle$ is said to be **entangled** if its Schmidt rank is greater than 1.

It is said to be **unentangled** otherwise.



$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \psi_{ij} & \end{bmatrix} \end{array}$$

Because $|\psi\rangle$ is a unit vector, the squares of its singular values are nonnegative real numbers that sum to 1. (**Exercise**!)

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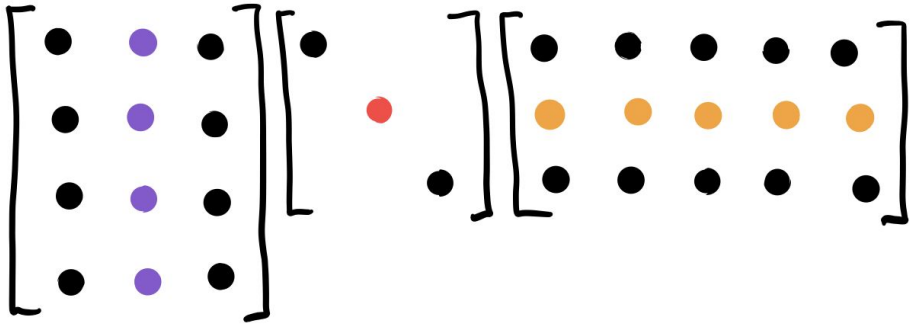

$$|\psi\rangle \longrightarrow M_\psi = \begin{array}{cc} & j \\ i & \begin{bmatrix} & \vdots & \\ \cdots & \psi_{ij} & \\ & & \end{bmatrix} \end{array}$$

Because $|\psi\rangle$ is a unit vector, the squares of its singular values are nonnegative real numbers that sum to 1. (**Exercise**!)

So we can consider the Shannon entropy of this probability distribution. This is called the **entanglement entropy** of $|\psi\rangle$.

$$-\sum_{i=1}^{\mathrm{rank}(M_\psi)} \sigma_i^2 \log(\sigma_i^2)$$

The number of non-zero singular values is called the **Schmidt rank** of the quantum state $|\psi\rangle$. It is a measure of entanglement between the two subsystems.

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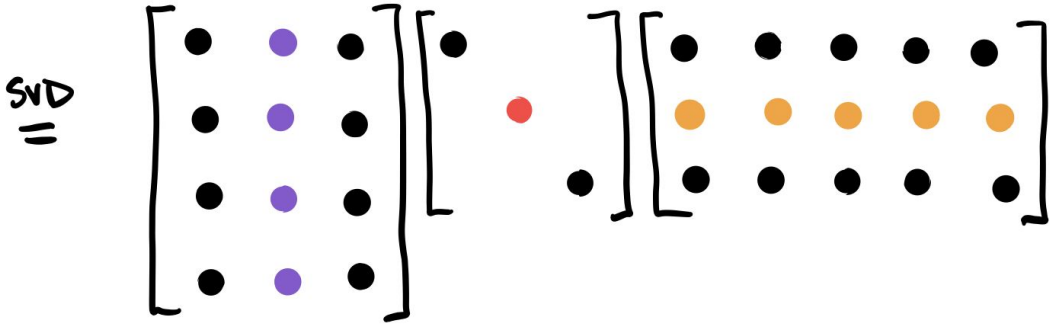


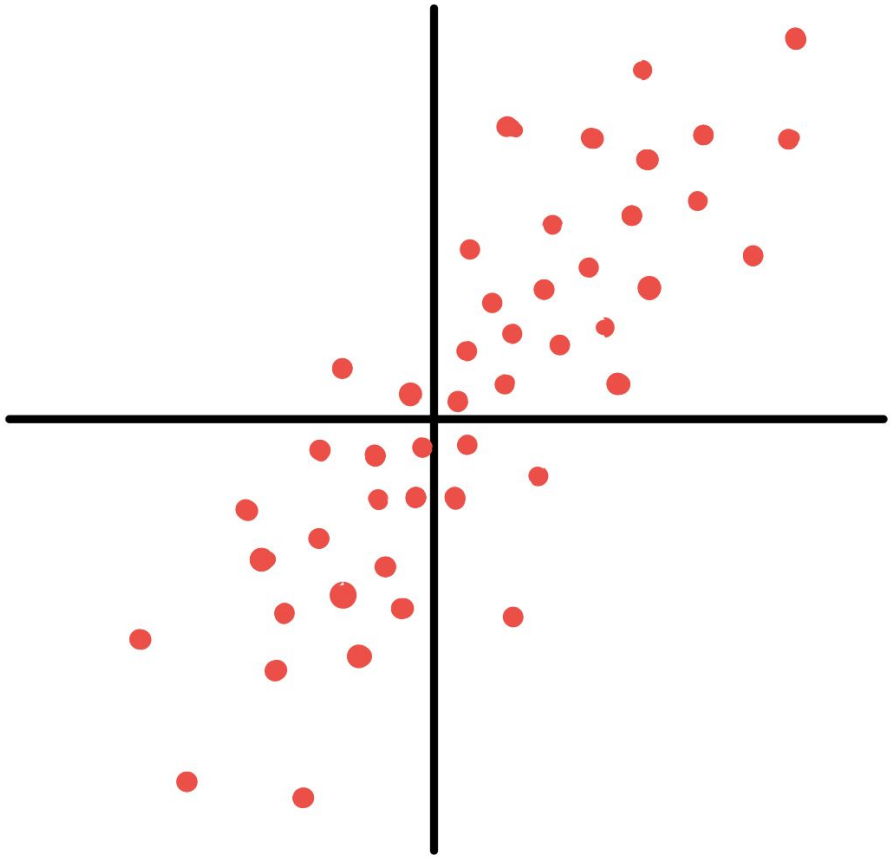
Okay. What else?

Another answer: PCA

Suppose we have n data points in m-dimensional space.

Oftentimes, these points may be **clustered** along a line or other low-dimensional subspace.

What is that line or subspace?



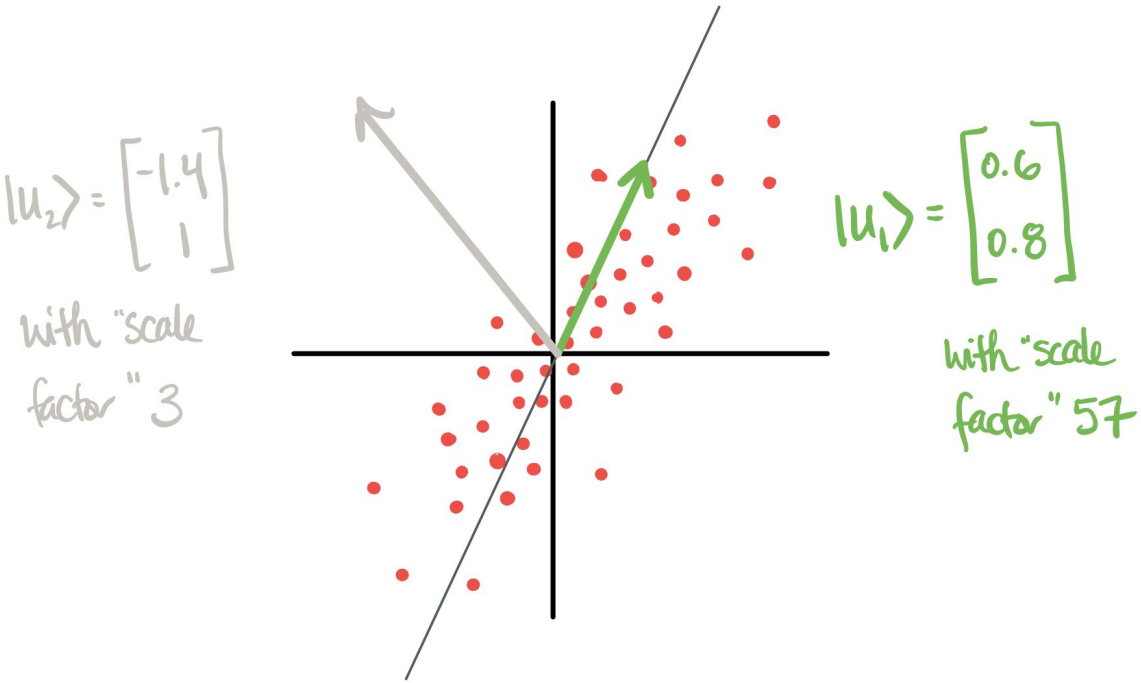
To find this line, first organize the data points into an $m \times n$ matrix A, and then compute the eigenvectors of $AA^T/n\text{-}1$.

Exercise: Convince yourself that AA^T is Hermitian!

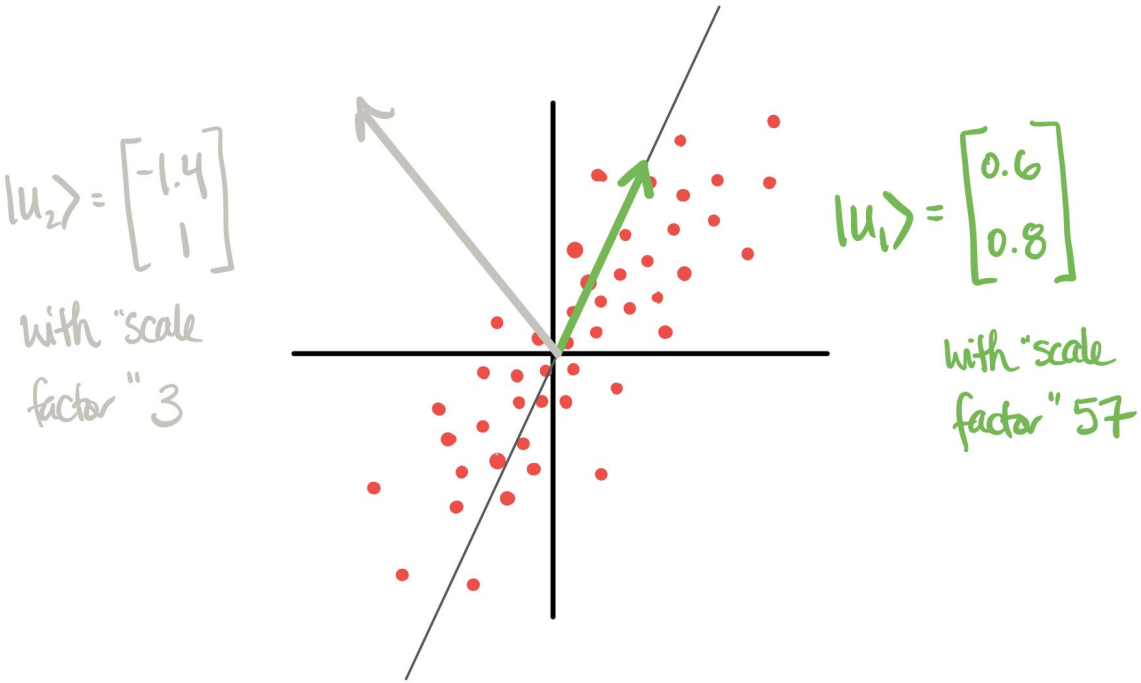
$$
\begin{array}{cc}
 & \begin{array}{cccccc} \text{student 1} & \text{student 2} & \text{student 3} & \text{student 4} & \text{student 5} & \text{student 6} \end{array} \\
A = & \begin{bmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{bmatrix} \begin{array}{l} \text{math} \\ \text{history} \end{array}
\end{array}
$$

There's a little more to this. We first center the data points by subtracting the *mean* of each row. The matrix $AA^T/n\text{-}1$ is called a *sample covariance matrix*.

In this example, the matrix $AA^T/5$ has two eigenvectors, shown below. The eigenvector with the largest eigenvalue picks out the **principal direction** of the data.



This is the idea behind **principal component analysis** (PCA). For more on this example, see ch. 7 of Gilbert Strang's *Introduction to Linear Algebra*, 5th ed.



Exercises

Exercises

1. The following three matrices are called the **Pauli matrices.**

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

   a. Show that the Pauli matrices are Hermitian and unitary.
   b. Find the eigenvalues and eigenvectors of each Pauli matrix.

2. A linear operator P is called a **projection operator** if $P^2 = P$.
   a. Show that the eigenvalues of a projection operator are 0 or 1.
   b. Show that $P = |\psi\rangle\langle\psi|$ is a projection for any unit vector $|\psi\rangle$.

3. Prove that all eigenvalues of a Hermitian matrix are real numbers. Prove that all eigenvalues of a unitary matrix have modulus 1, that is, can be written as $e^{i\theta}$ for some real number θ.

Exercises

4. A square $n \times n$ matrix M is called **positive semidefinite** (PSD) whenever $\langle v|M|v\rangle \geq 0$ for all vectors $|v\rangle$ in $\mathbb{C}^n$.
   a. Show that every Hermitian projection operator is PSD.
   b. Show that the eigenvalues of a PSD operator are always nonnegative.
   c. Show that $A^\dagger A$ is PSD for any operator A.

5. A square matrix $M: \mathbb{C}^n \longrightarrow \mathbb{C}^n$ is called **diagonalizable** if there is an invertible matrix U and diagonal matrix D so that $D = U^{-1}MU$, in which case D is called a **diagonal representation** of M. Find a diagonal representation of the Pauli matrix X.

Break

(10 min.)

Solution Walk-Through

(10 min.)

Solution #3.

FACT: If $M|v\rangle = \lambda|v\rangle$, then

$$\left(M|v\rangle\right)^{+} = \left(\lambda|v\rangle\right)^{+} \quad \text{ie} \quad \langle v|M^{+} = \bar{\lambda}\langle v|.$$

Now suppose M is Hermitian, $M^{+} = M$.

Solution #3.

$$M|v\rangle = \lambda|v\rangle \quad \Longleftrightarrow$$

"Hermitian operators
have real
eigenvalues."

Solution #3.

$$M|v\rangle = \lambda|v\rangle \iff \langle v|M|v\rangle = \lambda\langle v|v\rangle$$

$$\iff$$

"Hermitian operators have real eigenvalues."

Solution #3.

$$M|v\rangle = \lambda|v\rangle \iff \langle v|M|v\rangle = \lambda\langle v|v\rangle$$

$$\iff \langle v|M^{+}|v\rangle = \lambda\langle v|v\rangle$$

$$\iff$$

"Hermitian operators have real eigenvalues."

Solution #3.

$$M|v\rangle = \lambda|v\rangle \iff \langle v|M|v\rangle = \lambda\langle v|v\rangle$$

$$\iff \langle v|M^{+}|v\rangle = \lambda\langle v|v\rangle$$

$$\iff \bar{\lambda}\langle v|v\rangle = \lambda\langle v|v\rangle$$

$$\iff$$

"Hermitian operators have real eigenvalues."

Solution #3.

$$M|v\rangle = \lambda|v\rangle \iff \langle v|M|v\rangle = \lambda\langle v|v\rangle$$

$$\iff \langle v|M^{+}|v\rangle = \lambda\langle v|v\rangle$$

"Hermitian operators have real eigenvalues."

$$\iff \bar{\lambda}\langle v|v\rangle = \lambda\langle v|v\rangle$$

$$\iff \bar{\lambda} = \lambda$$

$$\iff \lambda \text{ is real.}$$

Solution #3.

Suppose $\mathcal{U}$ is unitary. Then

$$\mathcal{U}|v\rangle = \lambda|v\rangle \iff$$

"Unitary operators have eigenvalues with modulus 1."

Solution #3.

Suppose $\mathcal{U}$ is unitary. Then

$$\mathcal{U}|v\rangle = \lambda|v\rangle \iff \langle v|\mathcal{U}^\dagger\mathcal{U}|v\rangle = \lambda\langle v|\mathcal{U}^\dagger|v\rangle$$

$$\iff$$

"Unitary operators have eigenvalues with modulus 1."

Solution #3.

Suppose $\mathcal{U}$ is unitary. Then

$$\mathcal{U}|v\rangle = \lambda|v\rangle \iff \langle v|\mathcal{U}^\dagger\mathcal{U}|v\rangle = \lambda\langle v|\mathcal{U}^\dagger|v\rangle$$

$$\iff \langle v|I|v\rangle = \lambda\bar{\lambda}\langle v|v\rangle$$

$$\iff$$

"Unitary operators have eigenvalues with modulus 1."

Solution #3.

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$$\iff \langle v|I|v\rangle = \lambda\bar{\lambda}\langle v|v\rangle$$

$$\iff \langle v|v\rangle = |\lambda|\langle v|v\rangle$$

$$\iff 1 = |\lambda|$$

$$\iff \lambda = e^{i\theta}, \quad \theta \in \mathbb{R}.$$

"Unitary operators have eigenvalues with modulus 1."

Solution #5.

"The Pauli matrix X is diagonalizable."

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Solution #5.

X has eigenvectors & eigenvalues (check!)

$$|+\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, \lambda_+ = 1 \quad \& \quad |-\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}, \lambda_- = -1$$

"The Pauli matrix X is diagonalizable."

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Solution #5.

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"The Pauli matrix X is diagonalizable."

By the spectral theorem,

$$X = |+\rangle\langle+| - |-\rangle\langle-|$$

$$X = \begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}$$

$$= \underbrace{\begin{bmatrix}1/\sqrt{2} & 1/\sqrt{2}\\1/\sqrt{2} & -1/\sqrt{2}\end{bmatrix}}_{U}\underbrace{\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}}_{D}\underbrace{\begin{bmatrix}1/\sqrt{2} & 1/\sqrt{2}\\1/\sqrt{2} & -1/\sqrt{2}\end{bmatrix}}_{U^{-1}}$$

Solution #5.

and so $X = UDU^{-1}$ implies

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = D = UXU^{-1}.$$

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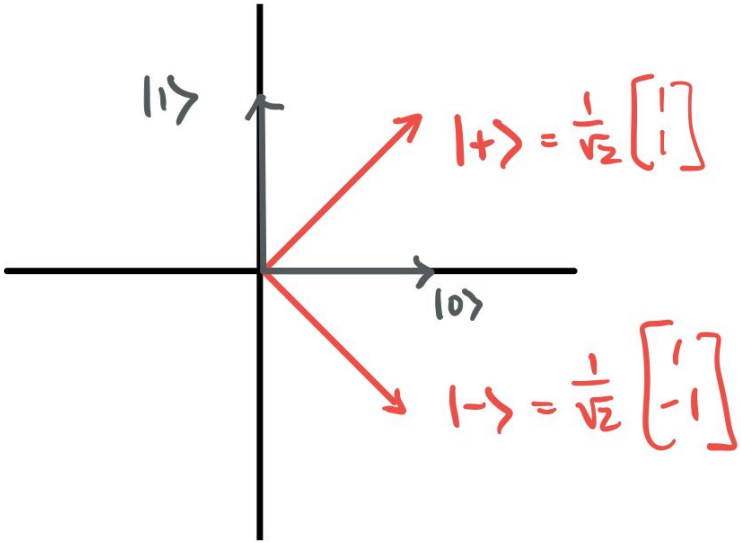

= old basis in which $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ is <u>not</u> diagonal.

= new basis in which "$X = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$" <u>is</u> diagonal.

Thank you!