ESQC 2024

Mathematical Methods Lecture 2

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Where to find the material

SCAN ME

- Alternative 1:
  - www.esqc.org, go to“lectures”
  - Find links there
- Alternative 2:
  - Scan QR code
  - simenkva.github.io/esqc_material

Matrices

We pick up from last time

Matrices = linear transformations

$$A(\mathbf{x})_i = \sum_{j=1}^{n} A_{ij} x_j$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}$$

$$A(\mathbf{x}) = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Space of matrices

- A matrix is a table

rows

cols

$$A \in \mathbb{F}^{m \times n} = M(m, n; \mathbb{F})$$

$$m \left\{ A = \overbrace{\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix}}^{n} \right.$$

- Vectors are also matrices!

$$\mathbf{x} \in \mathbb{F}^{n} = \mathbb{F}^{n \times 1} = M(n, 1; \mathbb{F})$$

Matrix—matrix product

- $C(\mathbf{x}) = A(B(\mathbf{x}))$ is a linear transformation, too.

Definition : Matrix product

Let $A \in M(n, m, \mathbb{F})$ and $B \in M(m, o, \mathbb{F})$. Then the *matrix product* $C = AB \in M(n, o; \mathbb{F})$ is defined by the formula

$$C_{ik} = \sum_{j=1}^{n} A_{ij} B_{jk}. \tag{1}$$

The matrix product satisfies:

1. $A(BC) = (AB)C$ ***associativity***
2. $(A + B)C = AC + BC$ and $A(B + C) = AB + AC$ ***distributivity***

However, the matrix product is *not commutative*, i.e., $AB \neq BA$ in general!

Computing the matrix product

$$AB = C \qquad C_{ij} = \sum_k A_{ik} B_{kj}$$

$$\begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1o} \\ B_{21} & B_{22} & \cdots & B_{2o} \\ \vdots & \vdots & \ddots & \vdots \\ B_{n1} & B_{n2} & \cdots & B_{no} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1o} \\ C_{21} & C_{22} & \cdots & C_{2o} \\ \vdots & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \cdots & C_{mo} \end{bmatrix}$$

Also, since $\mathbf{x}$ is a matrix, we write

$$A(\mathbf{x}) = A\mathbf{x}$$

Important matrix operations

- *Transpose:*

$$(A^T)_{ij} = A_{ji} \qquad \begin{bmatrix} 0 & 1 \\ \mathrm{i} & 2 \\ 0 & -1 \end{bmatrix}^T = \begin{bmatrix} 0 & \mathrm{i} & 0 \\ 1 & 2 & -1 \end{bmatrix}$$

- *Hermitian adjoint:*

$$(A^H)_{ij} = \overline{A_{ji}} \qquad \begin{bmatrix} 0 & 1 \\ \mathrm{i} & 2 \\ 0 & -1 \end{bmatrix}^H = \begin{bmatrix} 0 & -\mathrm{i} & 0 \\ 1 & 2 & -1 \end{bmatrix}$$

- *Inner product as matrix product:*

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^H \mathbf{y}$$

$$\begin{bmatrix} \cdots & \mathbf{x}^H & \cdots \end{bmatrix} \begin{bmatrix} \vdots \\ \mathbf{y} \\ \vdots \end{bmatrix}$$

More on matrices

Matrices are very central to quantum chemistry and numerical methods in general

Examples of matrices working in 2D Euclidean space

- Show Jupyter notebook
  - Lecture 2 – plane transformations.ipynb
- Examples of: rotation, reflection, scaling

The structure of a matrix

- A matrix has a set of *columns*

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n]$$

- What happens if we compute $A\mathbf{x}$?

$$A\mathbf{x} = \sum_{i=1}^{n} \mathbf{a}_i x_i$$

A linear combination of the columns

Definition : Column space

For a matrix $A = [\mathbf{a}_1, \cdots, \mathbf{a}_n] \in \mathbb{F}^{n\times m}$, the *column space* is the set of all linear combinations of the columns $\mathbf{a}_i$. This is also denoted *the range* or *image* of A, since it is the set of all vectors $A\mathbf{x}$.

The column space is a linear vector space, written

$$\operatorname{span}\{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n\}. \tag{1}$$

The *rank* of the matrix is the dimension of the column space. (It is a fact that the dimension of the row space is the same as the dimension of the column space.)

The row space is defined similarly.

Example

- What is the column space of the identity matrix?
- The columns are the standard basis vectors – a basis for $\mathbb{F}^3$
- $\cdots$ so the column space should be $\mathbb{F}^3$ as well!

$$\mathbb{1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \in \mathbb{F}^{3\times 3} \qquad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \mathbf{e}_1 x_1 + \mathbf{e}_2 x_2 + \mathbf{e}_3 x_3 = \mathbf{x}$$

Arbitrary in $\mathbb{F}^3$

Systems of linear equations

A main problem in linear algebra

- Let $A \in \mathbb{F}^{n \times n}$
- System of linear equations:

$$
\begin{aligned}
A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n &= y_1 \\
A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n &= y_2 \\
&\vdots \\
A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nn}x_n &= y_n
\end{aligned}
$$

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

- When does this system have a unique solution?
- Answer: When the matrix has rank n / col. space is a basis

Gaussian elimination

- A method for solving linear systems
- Read about it in the lecture notes!
- Or watch some high-quality videos, e.g. https://www.youtube.com/watch?v=2GKESu5atVQ (MyWhyU)

Inverse matrix

- Existence of unique solution gives *inverse matrix*

$$A\mathbf{x} = \mathbf{y} \qquad \Longleftrightarrow \qquad \mathbf{x} = A^{-1}\mathbf{y}$$

$$AA^{-1} = A^{-1}A = \mathbb{1}$$

- *Example: Inverse of plane rotation matrix*

$$\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}^{-1} = \begin{bmatrix} \cos(-\theta) & \sin(-\theta) \\ -\sin(-\theta) & \cos(-\theta) \end{bmatrix}$$

Inverse given by opposite rotation!

- Non-existence: *Singular matrix A.*

Example cont.

$$\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} =$$

$$\begin{bmatrix} \cos^2\theta + \sin^2\theta & -\cos\theta\sin\theta + \sin\theta\cos\theta \\ -\sin\theta\cos\theta + \cos\theta\sin\theta & \sin^2\theta + \cos^2\theta \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Special classes of matrices

Definition : Hermitian operator/matrix

A matrix $A \in M(n, n; \mathbb{F})$ is *Hermitian* if, for all $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$,

$$\langle \mathbf{x}, A\mathbf{y} \rangle = \langle A\mathbf{x}, \mathbf{y} \rangle, \quad \text{equivalently} \quad A^H = A. \tag{1}$$

$$H = \begin{bmatrix} 2 & 1+i & 3-2i \\ 1-i & 4 & 2+i \\ 3+2i & 2-i & 5 \end{bmatrix}$$

What's so special about Hermitian A?

- Only Hermitian operators have *real diagonal matrix elements*

$$\mathbf{u}^H A \mathbf{u} \quad \text{is always real}$$

- In quantum mechanics, *observables* are modelled with operators.
- Expectation value:

$$\mathbb{E}[A] := \frac{\mathbf{u}^H A \mathbf{u}}{\mathbf{u}^H \mathbf{u}} \quad \text{must be real}$$

- Thus observables must be Hermitian!

U
preserves
angles!

Definition : Unitary operator/matrix

A matrix $U \in M(n, n; \mathbb{F})$ is *unitary* if, for all $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$,

$$\langle U\mathbf{x}, U\mathbf{y}\rangle = \langle \mathbf{x}, \mathbf{y}\rangle\,, \quad \text{equivalently} \quad U^H U = U U^H = \mathbb{1}. \tag{1}$$

What characterizes a unitary matrix?

- U is unitary if and only if the columns are orthonormal

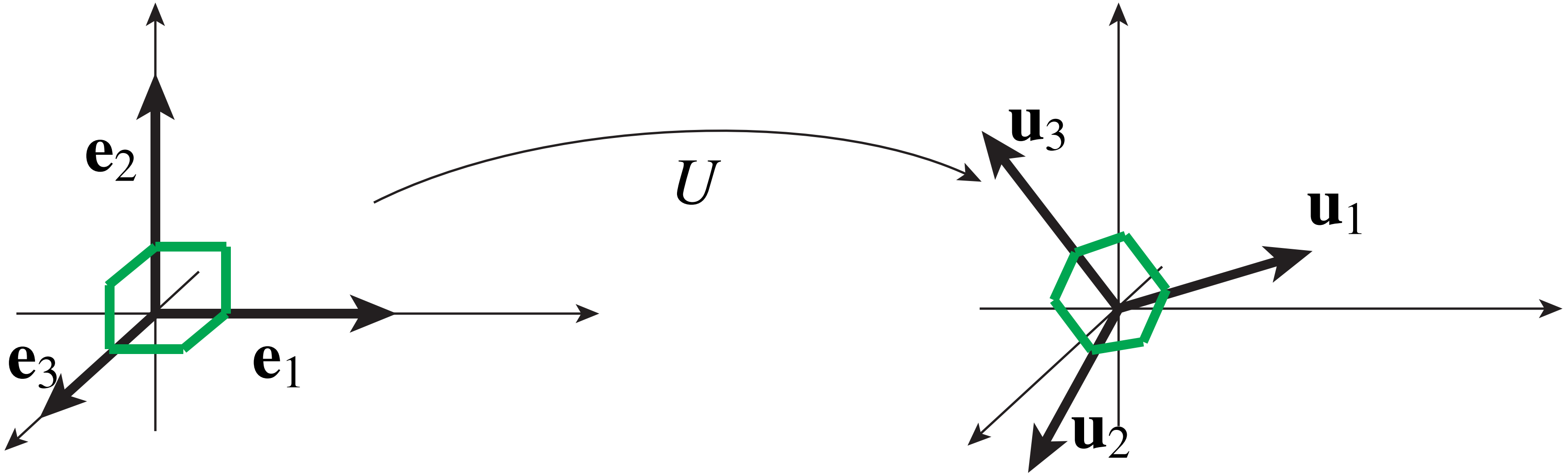
$$U = \begin{bmatrix} U_{11} & \cdots & U_{1i} & \cdots & U_{1n} \\ U_{21} & \cdots & U_{2i} & \cdots & U_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ U_{n1} & \cdots & U_{1i} & \cdots & U_{nn} \end{bmatrix} = [\mathbf{u}_1, \cdots, \mathbf{u}_i, \cdots, \mathbf{u}_n]$$

$$(U^H U)_{ij} = \mathbf{u}_i^H \mathbf{u}_j = \delta_{ij}$$

What does a unitary matrix do?

- U changes basis from standard basis to arbitrary orthonormal basis

$$U\mathbf{e}_i = \begin{bmatrix} U_{11} & \cdots & U_{1i} & \cdots & U_{1n} \\ U_{21} & \cdots & U_{2i} & \cdots & U_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ U_{n1} & \cdots & U_{ni} & \cdots & U_{nn} \end{bmatrix} \begin{bmatrix} 0 \\ \vdots \\ \boxed{1_i} \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} U_{1i} \\ U_{2i} \\ \vdots \\ U_{ni} \end{bmatrix} = \mathbf{u}_i$$



Example

- Rotation matrix

$$\begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix}^{-1} = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}$$

Matrix decompositions

Useful tools for characterizing and solving problems

Eigenvalue equation

Here posed as an "abstract" equation in Hilbert space

- Central equation of quantum chemistry:

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

- When a *basis* is introduced:

$$H\mathbf{u} = E\mathbf{u}$$

Matrix eigenvalue problem (EVP)

- Can we find solutions? How many solutions?

Theorem : Spectral theorem for Hermitian operators

Suppose $A \in \mathbb{F}^{n\times n}$ is Hermitian, i.e., $A^H = A$. Then, there exists an orthonormal basis $\{\mathbf{u}_1, \cdots, \mathbf{u}_n\}$, and real numbers $\{\lambda_1, \cdots, \lambda_n\}$, such that

$$H\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

Equivalently,

$$A = \sum_{i=1}^{n} \mathbf{u}_i \lambda_i \mathbf{u}_i^H = U \Lambda U^H$$

where $\mathbf{u}_i$ is the ith column of U, and where Λ is a diagonal matrix with elements $\Lambda_{ij} = \lambda_i \delta_{ij}$.

Theorem : Singular value decomposition

Let $A \in M(n, m, \mathbb{F})$ be a matrix, and let $k = \min(n, m)$. There exists k *singular values* $\sigma_i \geq 0$ and k *left singular vectors* $\mathbf{u}_i$, and k *right singular vectors* $\mathbf{v}_i$, such that

$$A = \sum_{i=1}^{k} \mathbf{u}_i \sigma_i \mathbf{v}_i^H = U \Sigma V^H,$$

POWERFUL!

where $U = [\mathbf{u}_1, \cdots, \mathbf{u}_k]$, $V = [\mathbf{v}_1, \cdots, \mathbf{v}_k]$, $\Sigma = \mathrm{diag}(\sigma_1, \cdots, \sigma_k)$. Equivalently,

$$A\mathbf{v}_i = \sigma_i \mathbf{u}_i.$$

The rank of A is the number of nonzero singular values. The decomposition is unique if all the singular values are distinct.

Example

- For example, useful for *approximations of matrices*
- Show Jupyter notebook with SVD of bitmap image

General finite-dimensional vector spaces

With several examples

Space of polynomials

A basis, but no longer Euclidean space

dimension

$$P_n = \left\{ f : [0,1] \to \mathbb{C} \mid f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n,\ \mathbf{a} \in \mathbb{C}^{n+1} \right\}$$

- Polynomials of degree $\leq n$
- A simple *function space*
- Show: Jupyter notebook
- Differentiation operator ($n = 4$)

derivative as a matrix!

$$\hat{D} x^i = i x^{i-1} \qquad D_{ji} = i\delta_{j,i-1}, \qquad D = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 4 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Space of matrices

- The space $M(n)$ of *square matrices (over some field)* is a vector space

$$(A+B)_{ij} = A_{ij} + B_{ij}, \quad (\alpha A)_{ij} = \alpha A_{ij}$$

- It is equal to $\mathbb{F}^m$, $m = n^2$ dimensions
- But we have an *additional structure:*

$$A, B \in M(n) \implies C = AB \in M(n)$$

- Vector space with vector-vector multiplication = *algebra*

A finite-dimensional C*-algebra

- In the second-quant lectures,

$$c_\ell \qquad c_k^\dagger \qquad \{c_\ell, c_k^\dagger\} = \delta_{\ell k}$$

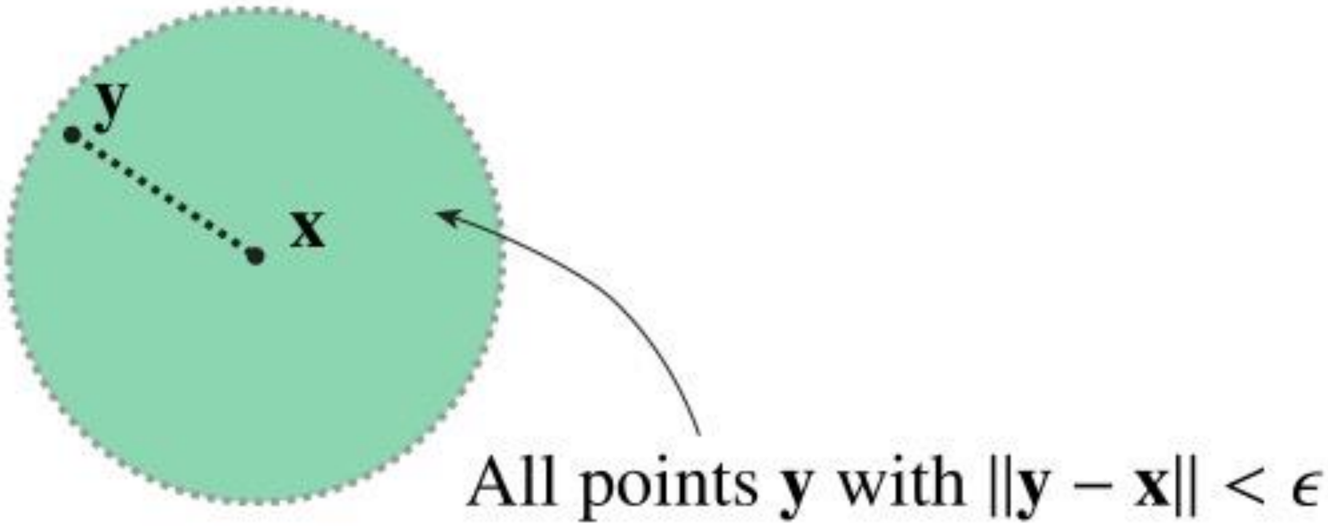
- We can consider an operator which is *a polynomial*

$$\alpha_0 \mathbb{1} \qquad + \sum_k \alpha_k c_k + \sum_k \beta_k c_k^\dagger$$
$$+ \sum_{k\ell} \alpha_{k\ell} c_k c_\ell + \sum_{k\ell} \beta_{k\ell} c_k^\dagger c_\ell + \sum_{k\ell} \gamma_{k\ell} c_k^\dagger c_\ell^\dagger$$

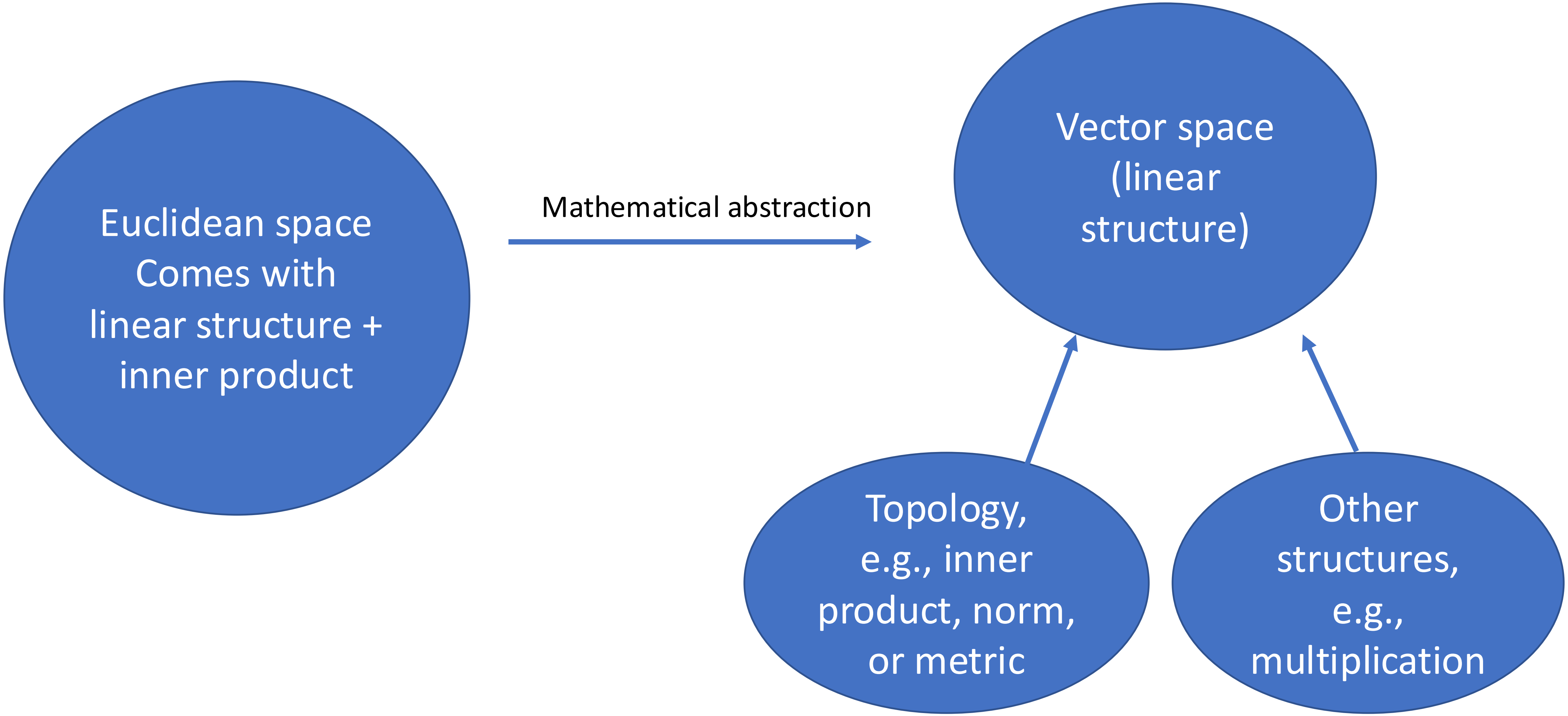
- If N spin-orbitals: max N particles, so max degree is $2N$
- So a finite dimensional vector space of operators
- Algebra: A vector space with a multiplication operation

Inner product, norm

- What these examples lack compared to Euclidean space:
  - A sense of distance
  - Euclidean space, as model of reality, comes with the intuition of which points are close to each other



General vector spaces



Definition : Vector space

A *vector space over the field* $\mathbb{F}$ is a set V together with a binary *vector addition* $+ : V \times V \to V$ and *scalar multiplication* $\cdot : \mathbb{F} \times V \to V$ such that, for all $x, y, z \in V$ and all $\alpha, \beta \in \mathbb{F}$, the following axioms are true:

1. There exists a $0 \in V$ such that $0 + x = x$ for all $x \in V$ ***identity element for addition***
2. $x + (y + z) = (x + y) + z$ ***associativity for addition***
3. $x + y = y + x$ ***commutativity for addition***
4. There exists x' such that $x +$ ***inverse element for addition***
5. $(\alpha\beta) \cdot x = \alpha \cdot (\beta \cdot x)$ ***scalar and field multiplications***
6. $1 \cdot x = x$ ***identity for scalar multiplication***
7. $(\alpha + \beta) \cdot x = \alpha \cdot x + \beta \cdot x$ ***distributivity of scalar multiplication***
8. $\alpha \cdot (x + y) = \alpha \cdot x + \alpha \cdot y$ ***distributivity of scalar multiplication***

Definition : Linear independence, dimension

Let V be a vector space, and $L \subset V$ a subset. The set L is *linearly indepdenent* if for any finite set $\{v_i \mid 1 \leq i \leq k\} \subset L$, we have

$$\sum_{i=1}^{k} a_i v_i = 0 \implies a_i = 0 \text{ for all } i$$

The *dimension* of V is the cardinality of the largest linearly independent subset of V.

- In Euclidean space: the *standard basis*
- Polynomials: the various x^i

Basis for finite-dimensional spaces

Definition : Basis

Let V be a vector space of finite dimension n. A basis is a linearly independent set of vectors $\{b_1, \cdots, b_n\}$, with exactly n elements.

Theorem

If $B = \{b_1, \cdots, b_n\}$ is a basis for a the vector space V, $\dim(V) < +\infty$, then any $v \in V$ can be uniquely decomposed as

$$v = \sum_{i=1}^{n} v_i b_i. \tag{1}$$

Example

- The standard basis in Euclidean space:

$$\mathbf{x} = \sum_{i=1}^{n} x_i \mathbf{e}_i$$

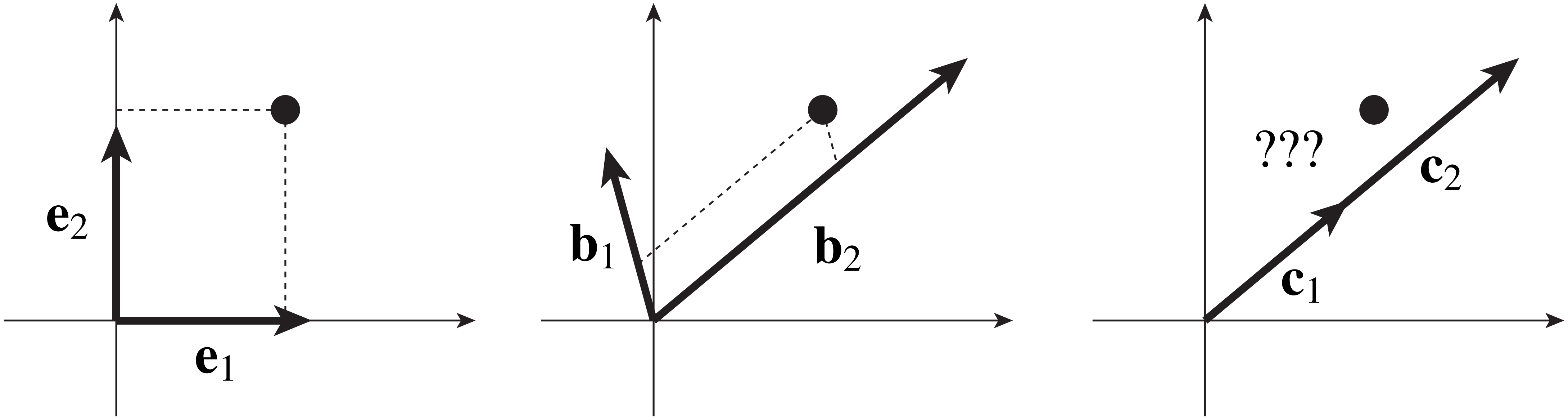
- The monomials in polynomial space:

$$p(x) = \sum_{i=0}^{n} a_i x^i$$

- A basis is *never unique*

Examples: bases in the plane

- Standard basis, non-orthogonal basis, and not-a-basis



Definition : Linear subspace

Let V be a vector space over $\mathbb{F}$. A subset $W \subset V$ is a *linear subspace* if it is closed under vector addition and scalar multiplication, i.e., if

$$\forall w \in W, \quad \alpha w \in W, \quad w_1 + w_2 \in W, \tag{1}$$

and if $0 \in W$.

- A line through the origin
- A plane through the origin
- Polynomials without constant terms
- Square integrable wavefunctions with finite kinetic energy

We will see this much later

All **finite** dimensional vector spaces are *isomorphic* – the same

- (… when it comes to the linear structure)

$$v = \sum_{i=1}^{n} x_i b_i \quad \longrightarrow \quad \mathbf{x} \in \mathbb{F}^n \qquad\qquad \alpha v = \sum_{i=1}^{n} \alpha x_i b_i \quad \longrightarrow \quad \alpha \mathbf{x} \in \mathbb{F}^n$$

$$v_1 + v_2 = \sum_{i=1}^{n} (x_{i1} + x_{i2}) b_i \quad \longrightarrow \mathbf{x}_1 + \mathbf{x}_2 \in \mathbb{F}^n$$

- And linear transformations become …. *matrices!*

$$\hat{A} v = \sum_{ij} A_{ij} x_j b_i$$

Action of
operator in the
given basis

Finite-dimensional Hilbert spaces

Definition : Inner product

Let V be a vector space. An *inner product* $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{F}$ is a map which satisfies the following axioms:

1. $\langle x, x \rangle \geq 0, \quad \langle x, x \rangle = 0$ if and only if $x = 0$ ***non-negative***
2. $\langle x, \alpha y + \beta z \rangle = \alpha \langle x, y \rangle + \beta \langle x, z \rangle$ ***linearity***
3. $\langle \alpha y + \beta z, x \rangle = \bar{\alpha} \langle y, x \rangle + \bar{\beta} \langle z, x \rangle$ ***conjugate linearity***
4. $\langle x, y \rangle = \overline{\langle y, x \rangle}$ ***hermiticity***

- Finite dim vector space + inner product = Hilbert space

All finite-dimensional Hilbert spaces are the same

- … when an orthonormal basis is selected
- Let V be a finite dim Hilbert space with given basis

$$\langle v, v' \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} \bar{x}_i \langle b_i, b_j \rangle x_j \equiv \mathbf{x}^H S \, \mathbf{x},$$

"overlap matrix"

- Inner prod *induces* an inner product on $\mathbb{F}^n$
- It is not the Euclidean inner product *unless*

$$\langle b_i, b_j \rangle = \delta_{i,j}, \quad \Longleftrightarrow \quad S = \mathbb{1}$$

Orthonormal basis

Remark

In order to study (the vector space structure of) finite dimensional Hilbert spaces, including the linear operators over these spaces, it suffices to study $\mathbb{F}^n$ and matrices $M(n, m, \mathbb{F})$.

End of lecture 2

- That’s it for today!