ESQC Mathematics Lecture 2

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Drop me a message!

Matrices

We pick up from last time

Quick recap: Linear operator as matrix

$$A(\mathbf{x})_i = \sum_{j=1}^{n} A_{ij} x_j \qquad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$

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

Space of matrices

- A matrix is a table

\# rows

\# cols

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

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

- 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 operator.

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

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

The matrix product satisfies:

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

However, them 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:*

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

- *Hermitian adjoint:*

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

- *Inner product as matrix product:*

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^H \mathbf{y} \qquad \begin{bmatrix} \cdots & \mathbf{x}^H & \cdots \end{bmatrix} \begin{bmatrix} \vdots \\ \mathbf{y} \\ \vdots \end{bmatrix}$$

General finite-dimensional vector spaces

With several examples

Space of polynomials

looks like a basis!

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 *function space*
- Show: Jupyter notebook
- Differentiation operator ($n = 4$)

we see that we get a matrix!

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

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 Euclidean space in 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 polynomi*

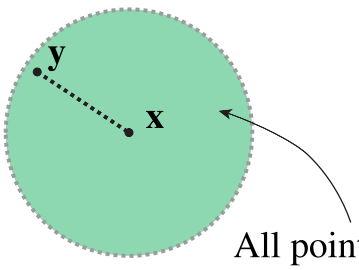
A very important example from the mathematical point of view

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

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

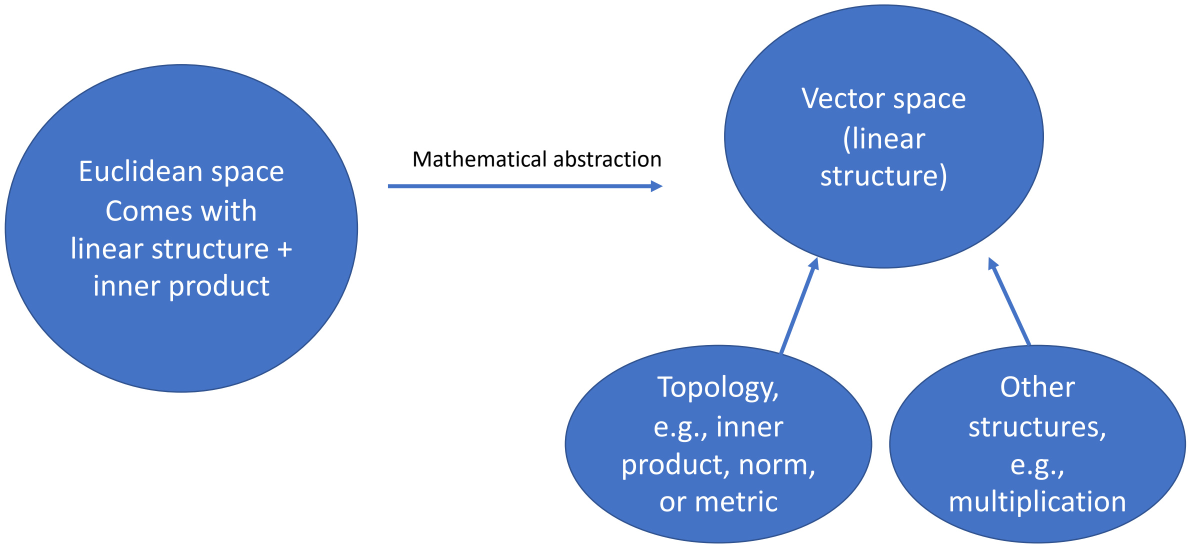
Inner product, norm

- 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



All points $\mathbf{y}$ with $\|\mathbf{y} - \mathbf{x}\| < \epsilon$

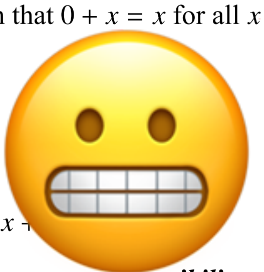
General vector spaces



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. $(\alpha\beta) \cdot x = \alpha \cdot (\beta \cdot x)$ — ***compatibility of 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

$$v = \sum_{i=1}^{n} v_i b_i. \quad (1)$$

Example

- The standard basis in Euclidean space:

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

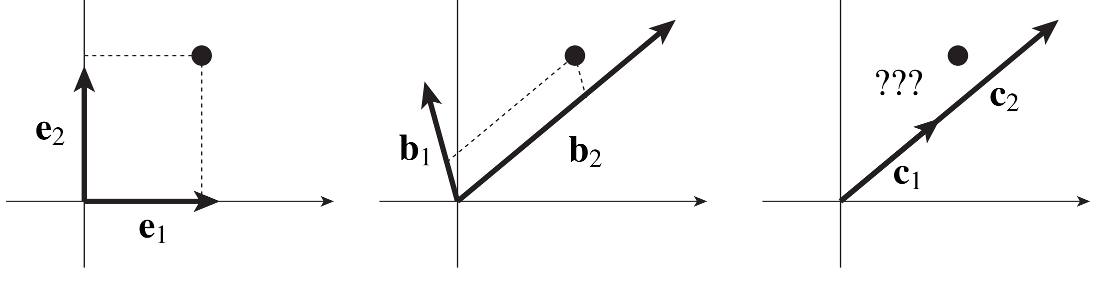
- The monomials in polynomial space:

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

- A basis is *never unique*

Examples: bases in the plane

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



Examples of infinite dimensions

- The space of *all* polynomials, unlimited degree
- The space of all *sequences*

$$\text{seq} = \{c : \mathbb{N} \to \mathbb{X}\}, \quad c = (c_0, c_1, c_2, \cdots)$$

- The space of *quadratically integrable functions*

$$\mathcal{L}^2(\mathbb{R}^N) = \left\{ f : \mathbb{R}^N \to \mathbb{C} \mid \int_{\mathbb{R}^N} |f(x)|^2 \, \mathrm{d}^N x < +\infty \right\}$$

Approximations of functions

For infinite basis expansions

Quantum mechanics!

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

- (… when it comes to the linear structure)

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

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

- And linear operators are …. *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 $\mathbb{F}^n$ and matrices $M(n, m, \mathbb{F})$.

More on matrices

Matrices are very central to finite dimensional spaces

Examples of matrices in 2D Euclidean space

- Show Jupyter notebook

End of lecture 2

- That's it for today!