ESQC Mathematics Lecture 3

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Drop me a message!

More on matrices

Matrices are very central to finite dimensional spaces

Examples of matrices working in 2D Euclidean space

- Show Jupyter notebook
- 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

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

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 $\mathbb{F}^3$
- ⋯ 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

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

A main problem in linear algebra

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

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

- 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)

Yes, almost everything is named after me, or should be

Inverse matrix

- Existence of unique solution gives *inverse matrix*

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

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

- *Example: Inverse of plane rotation matrix*

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

- Non-existence: *Singular matrix.*

From the "cat Jupyter notebook"

Inverse given by opposite rotation!

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 operators

Definition : Hermitian operator/matrix

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

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

Quantum mechanical Hamiltonian is Hermitian!

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 $\mathbf{x}, \mathbf{y} \in \mathbb{F}^n$,

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

What characterizes a unitary matrix?

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

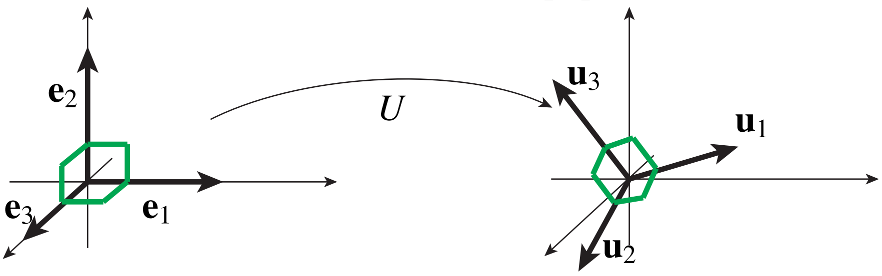
$$U = \begin{bmatrix} U_{11} & \cdots & U_{1i} & \cdots & U_{1n} \\ U_{21} & \cdots & U_{2i} & \cdots & U_{2n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ U_{n1} & \cdots & U_{1i} & \cdots & U_{nn} \end{bmatrix} = [\mathbf{u}_1, \cdots, \mathbf{u}_i, \cdots, \mathbf{u}_n]$$

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

What does a unitary matrix do?

- U changes basis from standard basis to arbitrary orthonormal basis

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



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

- Central equation of quantum chemistry:

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

Here posed as an "abstract" equation in Hilbert space

- 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

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

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.

POWERFUL!

Example

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

Vector calculus

Functions of several variables

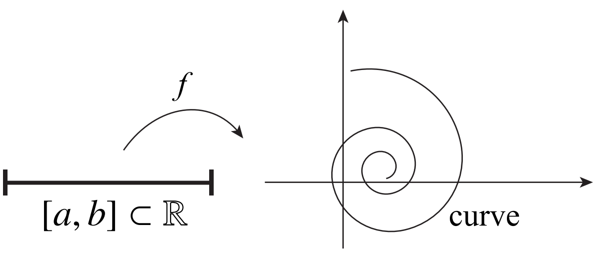
Functions of several variables

- We turn to the study of *vector valued* functions

$$f : \mathbb{R}^n \to \mathbb{R}^m \qquad f : \Omega(\subset \mathbb{R}^n) \to \mathbb{R}^m$$

- Paths

$$f : \Omega(\subset \mathbb{R}^1) \to \mathbb{R}^m$$



Scalar-valued

$$f : \Omega(\subset \mathbb{R}^n) \to \mathbb{R}^1$$

In quantum chemistry

One of the main reasons to study vector calculus

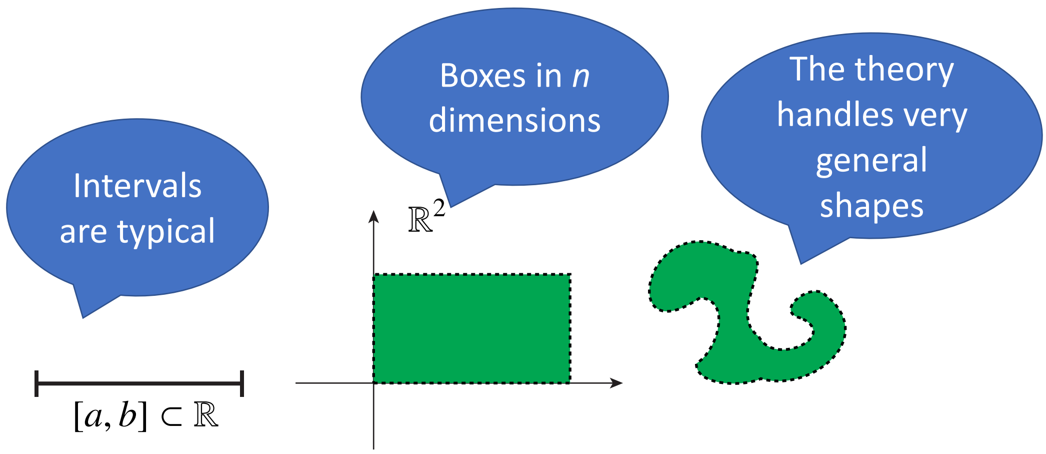
- *Most* methods can be formulated as:

$$E : \Omega(\subset \mathbb{F}^n) \to \mathbb{R}, \quad \mathbf{x} \mapsto \text{energy function}$$

Find $\mathbf{x} \in \Omega$ such that

$$E(\mathbf{x}) = \min!, \quad \text{i.e.,} \quad \nabla E(\mathbf{x}) = 0.$$

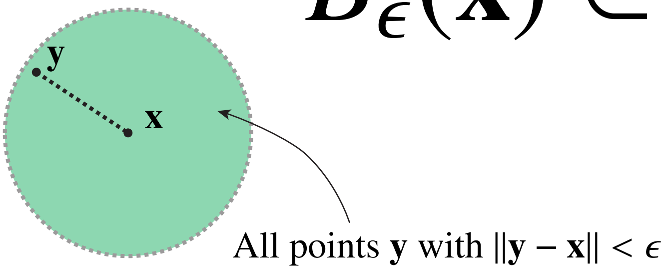
A typical domain Ω



Topology of Euclidean space

- Definition of an *epsilon-ball*

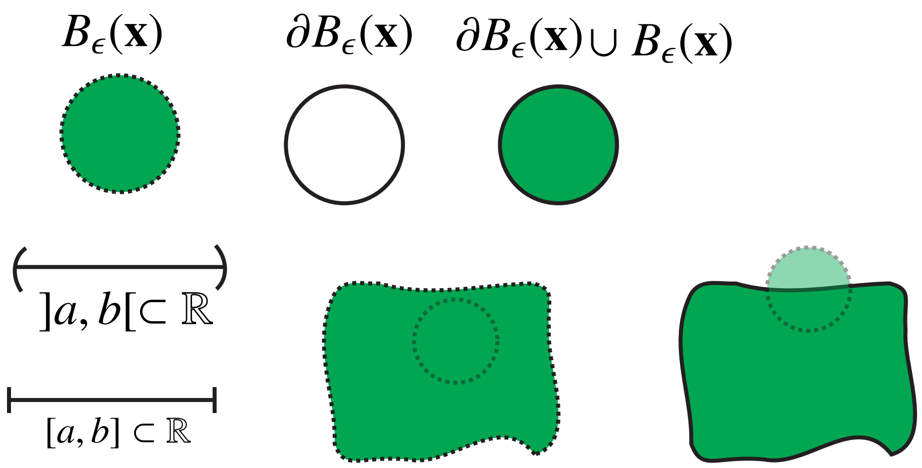
$$B_\epsilon(\mathbf{x}) \subset \mathbb{R}^n$$



Definition : Topologically important sets

1. A subset $S \subset \mathbb{R}^n$ is called *open* if, for every $\mathbf{x} \in S$, there is an $\varepsilon > 0$ such that $B_\varepsilon(\mathbf{x}) \subset S$.
2. A subset S is called *closed* if $S^{\complement} = \mathbb{R}^n \setminus S$ is open.
3. The *closure* $\text{cl}(S)$ is the smallest closed set that contains S.
4. The *interior* $\text{int}(S)$ is the set of all those $\mathbf{x} \in S$ around which there exists an ε-ball in S
5. The *boundary* ∂S is the intersection $\text{cl}(S^{\complement}) \cap \text{cl}(S) = S \setminus \text{int}(S)$

Examples



Definition : Limit

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$, where Ω is open. Let $\mathbf{x}_0 \in \Omega \cup \partial\Omega$, and let N be a neighborhood of $\mathbf{b} \in \mathbb{R}^m$.

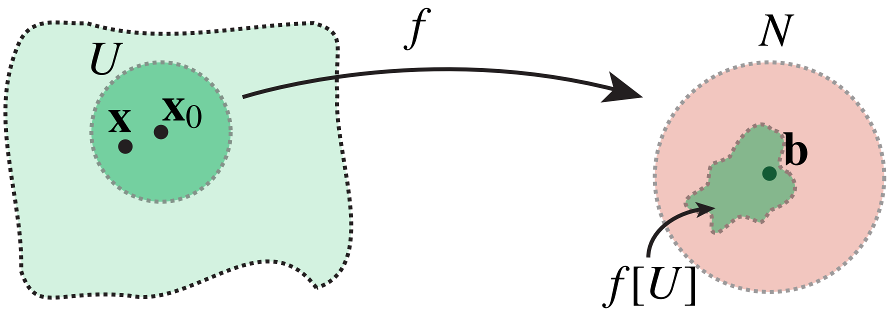
We say that f is *eventually in N as $\mathbf{x}$ approaches $\mathbf{x}_0$*, if there exists a neighborhood U of $\mathbf{x}_0$, such that $\mathbf{x} \in U$ but $\mathbf{x} \neq \mathbf{x}_0$ and $\mathbf{x} \in \Omega$ imply $f(x) \in N$.

We say that $f(\mathbf{x})$ *approaches* $\mathbf{b}$ *as* $\mathbf{x}$ *approaches* $\mathbf{x}_0$,

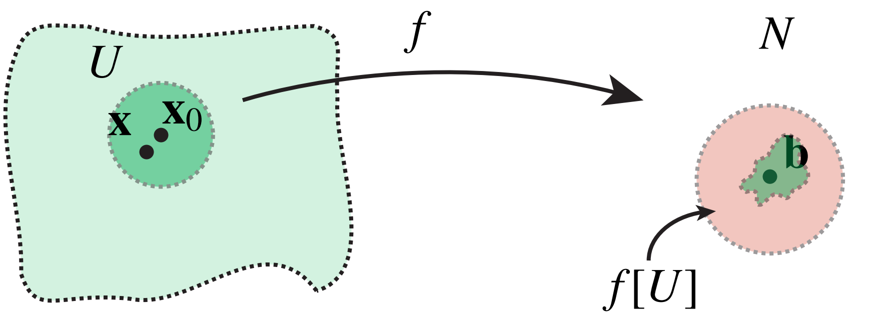
$$\lim_{\mathbf{x} \to \mathbf{x}_0} f(\mathbf{x}) = \mathbf{b} \quad \text{or} \quad f(\mathbf{x}) \to \mathbf{b} \text{ as } \mathbf{x} \to \mathbf{x}_0, \tag{1}$$

when, given any neighborhood N of $\mathbf{b}$, f is eventually in N as $\mathbf{x}$ approaches $\mathbf{x}_0$.

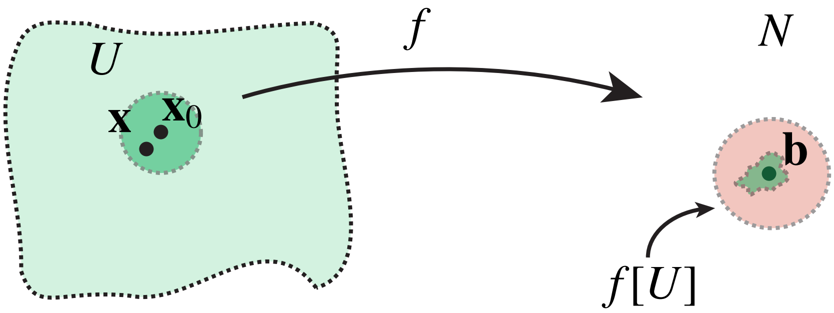
Intiuition



Intiuition



Intiuition



Definition : Continuity

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$. Let $\mathbf{x}_0 \in \Omega$. We say that f is *continuous at* $\mathbf{x}_0$ if

$$\lim_{\mathbf{x} \to \mathbf{x}_0} f(\mathbf{x}) = f(\mathbf{x}_0).$$

Multidimensional version of "unbroken graph"

Example

- Is the following function continuous at (0,0)?
- (Show notebook)

$$f : \mathbb{R}^2 \to \mathbb{R}, \quad (x, y) \mapsto \frac{x^2}{x^2 + y^2}$$

- No, because the limit does not exist.
- Different limit candidates if we approach from different directions
- *The definition of limit is designed to avoid this*

More subtle, in 1D

- Is the following function continuous?

$$f : (0, 1) \to \mathbb{R}, \quad x \mapsto \sin(1/x)$$

- Yes, at every x *in the interior of the domain*
- But f is discontinuous at the boundary point $x = 0$

Theorem : Properties of continuous functions

Let $f, g : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be functions with a common domain Ω, continuous at $\mathbf{x}_0$: Then:

1. $f + g$ and αf for any $\alpha \in \mathbb{R}$ are continuous at $\mathbf{x}_0$.
2. In the scalar-valued case $m = 1$, the product fg is continuous at $\mathbf{x}_0$
3. If $f \neq 0$ in all of Ω, then $1/f$ is continuous at $\mathbf{x}_0$
4. The component functions $f_i : \Omega \to \mathbb{R}$ are all continuous at $\mathbf{x}_0$. The converse is also true.

Theorem : Compositions of functions

Let $f : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ be continuous at $\mathbf{x}_0 \in \Omega$, and $g : \Omega' \subset \mathbb{R}^m \to \mathbb{R}^o$. Suppose $f[\Omega] \subset \Omega'$, and let g be continuous at $\mathbf{y}_0 = f(\mathbf{x}_0)$. Then $h : \Omega \subset \mathbb{R}^n \to \mathbb{R}^o$,

$$h(\mathbf{x}) = g(f(\mathbf{x}_0)$$

is continuous at $\mathbf{x}_0$.

These two theorems can be used to decide continuity of very complicated functions, once simpler functions are proven to be continuous

Examples

- polynomials in any variable
- exponential function
- sine, cosine …
- any composition

$$f : \mathbb{R}^3 \to \mathbb{R}, \quad f(\mathbf{x}) = \exp[-\|\mathbf{x}\|^4 + \cos(x_1)]x_1 x_2 x_3^4 (1 + x_1^2)^{-2}$$

End of lecture 3

- Next time, differentiable functions