

## AMAT 342 Lecture 15

- Finish with RMSD
- Return / review exams
- Topology of metric spaces.

Recall: RMSD:  $O^n \times O^n \rightarrow [0, \infty)$  is given by

$$\text{RMSD}(P, P') = \min_{\varphi \in E} \frac{1}{n} \sum d_2(V(P), V(\varphi(P'))).$$

*ordinary  
Euclidean  
distance*

where:  $O^n$  = Set of all length  $n$  ordered lists of points in  $\mathbb{R}^3$ .

$E$  = Set of all rigid motions of  $\mathbb{R}^3$

$V: O^n \rightarrow \mathbb{R}^{3n}$  is given by

$$V((x_1, y_1, z_1), (x_2, y_2, z_2), \dots, (x_n, y_n, z_n))$$

$$= (x_1, y_1, z_1, x_2, y_2, z_2, \dots, x_n, y_n, z_n).$$

RMSD satisfies properties 2 and 3 of a metric. [proof omitted]

Also  $\text{RMSD}(P, P) = 0$  if  $P \in O^n$ , because  $I_d|_{\mathbb{R}^3}: \mathbb{R}^3 \rightarrow \mathbb{R}^3$  is a rigid motion.

But we can have  $\text{RMSD}(P, Q) = 0$  but  $P \neq Q$ .

we saw an example of this last lecture,

$\Rightarrow$  property 1 of a metric does not hold.

Namely, let  $Q = \varphi(P)$  for any rigid motion  $\varphi$ .

Then  $\varphi^{-1}$  is a rigid motion, and

$$\begin{aligned} d_2(V(P), V(\varphi^{-1}(Q))) &= d_2(V(P), V(\varphi^{-1}(\varphi(P)))) \\ &= d_2(V(P), V(P)) = 0 \end{aligned}$$

so  $\text{RMSD}(P, Q) = 0$ .

We'll modify RMSD to get a metric.

Define an equivalence relation  $\sim$  on  $O^n$  by

$P \sim Q$  iff  $\exists$  a rigid motion  $\varphi: \mathbb{R}^3 \rightarrow \mathbb{R}^3$   
with  $\varphi(P) = Q$ .

\* Fact:  $\text{RMSD}(P, Q) = \text{RMSD}(P', Q')$  if  $P \sim P'$  and  
 $Q \sim Q'$   
(Exercise: Prove this).

As a consequence,  $\text{RMSD} : O^n \times O^n \rightarrow [0, \infty)$   
descends to a genuine metric on  $O^n / \sim$ .

Specifically, we define

$\overline{\text{RMSD}} : O^n / \sim \times O^n / \sim \rightarrow [0, \infty)$  by

$$\overline{\text{RMSD}}([P], [Q]) = \text{RMSD}(P, Q).$$

By the fact  $\star$ , this function is well defined.

Exercise: Prove that  $\overline{\text{RMSD}}$  is a metric.

Exam: Total points = 33 (Excludes 1 exam taken  
Mean = 23.1 a week later)  
Median = 22.25

Curve: Take the number of points you lost  
and multiply it by .43 That's the  
number of points you lost in the curved score.

curved mean  $\approx 87$ .

## Exam review

4. Prove that if  $f: S \rightarrow T$  and  $g: T \rightarrow U$  is a homeomorphism, then  $gof: S \rightarrow U$  is a homeomorphism.

Pf: Since  $f$  and  $g$  are homeomorphisms

$f$  and  $g$  are continuous,

$f^{-1}$  and  $g^{-1}$  are continuous,

$\Rightarrow gof$  is continuous and  $f^{-1} \circ g^{-1}$  is continuous.

(Composition of continuous functions is continuous).

Note that  $(gof)^{-1} = f^{-1} \circ g^{-1}$

$$(gof) \circ (f^{-1} \circ g^{-1}) = g \circ (f \circ f^{-1}) \circ g^{-1} = g \circ g^{-1} = \text{Id}_U.$$

$$(f^{-1} \circ g^{-1}) \circ (gof) = f^{-1} \circ (g^{-1} \circ g) \circ f = f^{-1} \circ f = \text{Id}_S.$$

Thus  $gof$  is invertible, hence a bijection.

6. Let

$$S = \{(1, y) \mid y \in I\} \subset \mathbb{R}^2$$

$$T = \{(2, y) \mid y \in I\} \subset \mathbb{R}^2$$

a Sketch S and T

b. Give an explicit homeomorphism  $f: S \rightarrow T$

$$f(1, y) = (2, y).$$

c. What is  $f^{-1}$ ?  $f^{-1}(2, y) = (1, y).$

d. Give an explicit expression for an isotopy

$$h: S \times \overline{I} \rightarrow \mathbb{R}^2 \text{ from } S \text{ to } T$$

$$h((1, y), t) = (1+t, y)$$

e. Is  $h$  invertible?

No.  $\text{im}(h) = [1, 2] \times I \Rightarrow h$  is not surjective  
 $\Rightarrow h$  is not a bijection  
 $\Rightarrow h$  is not invertible.

However,  $h$  can be "reversed" to give an isotopy  $\bar{h}$  from  $T$  to  $S$ :

$$\bar{h}: S \times \overline{I} \rightarrow \mathbb{R}^2, \bar{h}((1, y), t) = h((1, y), (1-t)) = (1+(1-t)y)$$

$$= ((2-t), y)$$

$\bar{h}$  is not an inverse of  $h$ .

7. Let  $T_k$  denote a subset of the unit circle obtained by removing  $k$  distinct points from  $S^1$ .

How many path components does  $T_k$  have?

Ans:  $k$ .

8. Prove that if  $f: S \rightarrow T$  is an embedding then  $S$  and  $\text{im } f$  have the same # of path components.

Pf:  $f$  is an embedding means that  $\tilde{f}: S \rightarrow \text{im}(f)$  is a homeomorphism, where  $\tilde{f}(x) = f(x) \neq x$ .

Proposition: homeomorphic spaces have the same # of path components.

$\Rightarrow S$  and  $\text{im}(f)$  have same # of path components

## Metrics and topology

Metric space definition of continuity:

Let  $M$  and  $N$  be metric spaces with metrics  $d_M, d_N$ .

A function  $f: M \rightarrow N$  is continuous at  $x \in M$  if  
 $\forall \epsilon > 0, \exists \delta > 0$  such that  
 $d_M(x, y) < \delta \Rightarrow d_N(f(x), f(y)) < \epsilon.$

$f$  is said to be continuous if it is continuous at each  $x \in M$ .

(This definition generalizes the definition for Euclidean subspaces considered earlier).

Example: Let  $M$  be any metric space and take  $N$  to be  $\mathbb{R}$  with the Euclidean metric.

For any  $x \in M$ , the function  $d^x: M \rightarrow \mathbb{R}$  given by  $d^x(y) = d_N(x, y)$  is a continuous function.

Pf: Exercise.

With this definition of continuity, the definition of homeomorphism extends immediately to metric spaces:

For metric spaces  $M$  and  $N$ ,

$f: M \rightarrow N$  is a homeomorphism if

- 1)  $f$  is a continuous bijection
- 2)  $f^{-1}$  is also continuous.

Example: Consider the metric  $d$  on  $[0, 2\pi]$  given by  $d(x, y) = \min(|x - y|, |(x + 2\pi) - y|, |(x - 2\pi) - y|)$



take  $S^1$  to have usual  
Euclidean metric

Then the function  $f: ([0, 2\pi], d) \rightarrow S^1$  given by  $f(t) = (\cos t, \sin t)$  is a homeomorphism.

The definition of isotopy also extends, but we'll not get into the details of this.

## An alternate description of continuity

### Open Sets

Let  $M$  be a metric space. For  $x \in M$  and  $r > 0$ , the open ball in  $M$  of radius  $r$ , centered at  $x$ , is the set

$$B(x, r) = \{y \in M \mid d_M(x, y) < r\}.$$

Example: For  $M = \mathbb{R}^2$  with the Euclidean distance,  $B(\vec{0}, 1)$  looks like this



disc of radius 1 centered at the origin, with the boundary not included.

For  $M = \mathbb{R}$ , the open ball of radius  $r$  centered at  $x$  is just the interval  $(x-r, x+r)$ .

A subset of  $M$  is called open if it is a union of (possibly infinitely many) open balls.

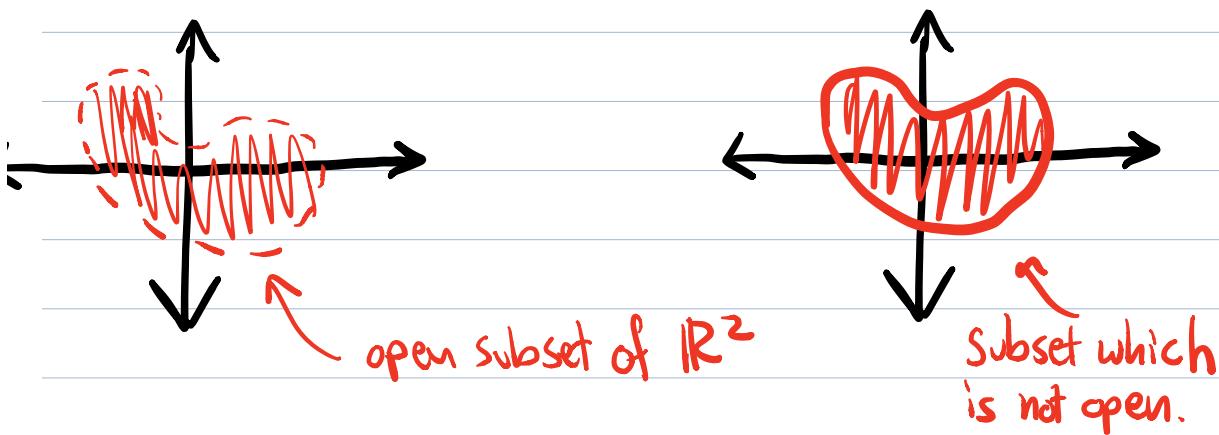
The empty set is always considered open.

$$M \text{ itself is open: } M = \bigcup_{x \in M} B(x, 1)$$

Fact: A region in  $\mathbb{R}^n$  is open if it contains none of its boundary points.

this is an informal statement because I haven't defined "boundary points." It can be made formal, but I will not go into the details.

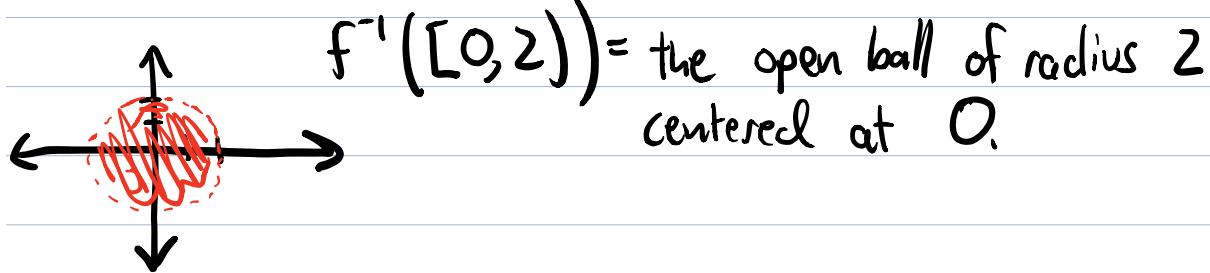
Illustration: Dashed line = boundary not included  
Solid line = boundary included



Fundamental Fact: Whether a function of metric spaces  $f: M \rightarrow N$  is continuous depends only on the open sets of  $M, N$  and not otherwise on the metric! (this is made precise by the proposition below)

Notation: For  $f: S \rightarrow T$  any function and  $U \subset T$ ,  $f^{-1}(U) = \{x \in S \mid f(x) \in U\}$ .

Example: Let  $f: \mathbb{R}^2 \rightarrow [0, \infty)$  be given by  
 $f(x) = d_2(x, 0)$ .



Proposition: A function  $f: M \rightarrow N$  of metric spaces is continuous if and only if  $f^{-1}(V)$  is open for every open subset of  $N$ .

Proof: Exercise.