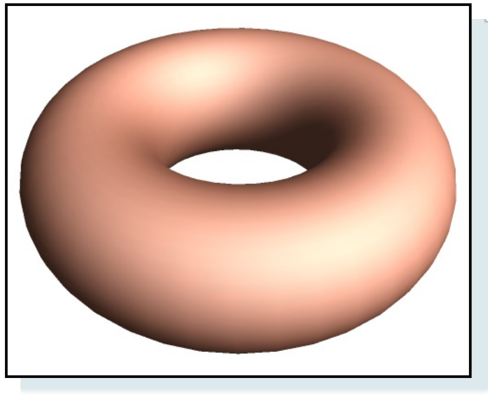
DSC 214
Topological Data Analysis

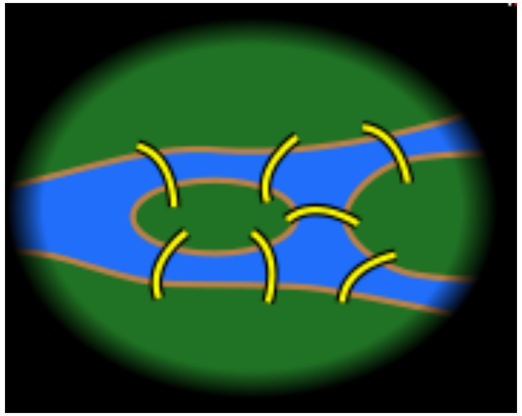
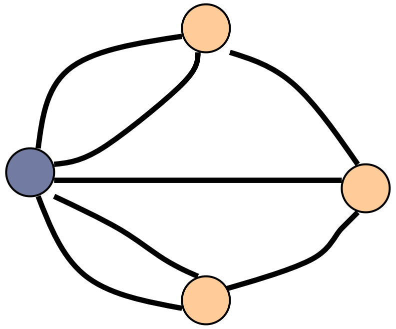
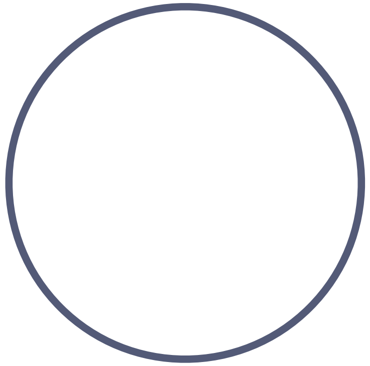
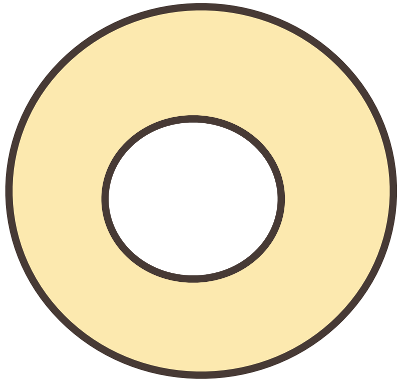
Topic 1: Basics

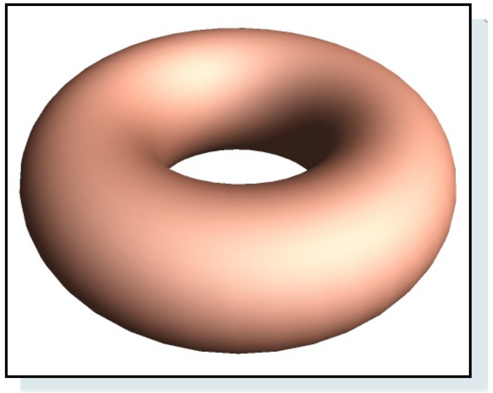
Instructor: Zhengchao Wan

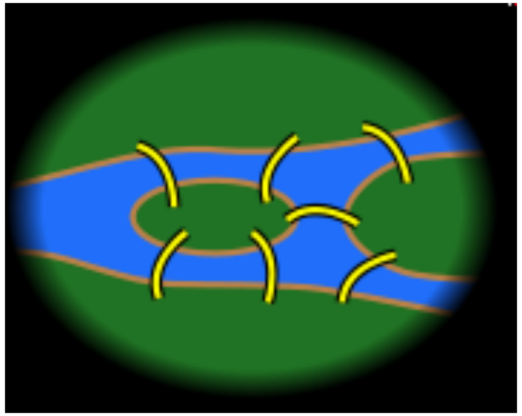
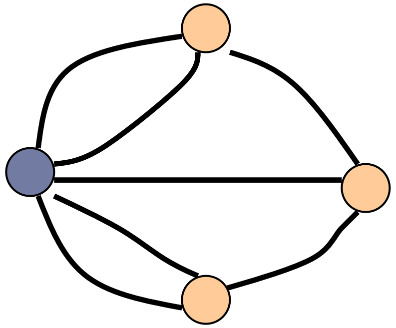
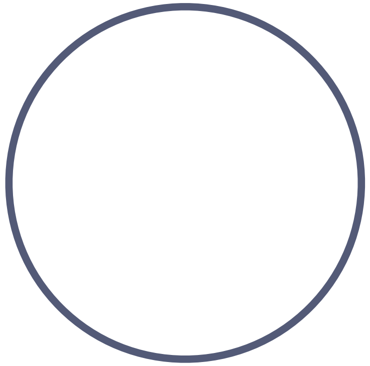
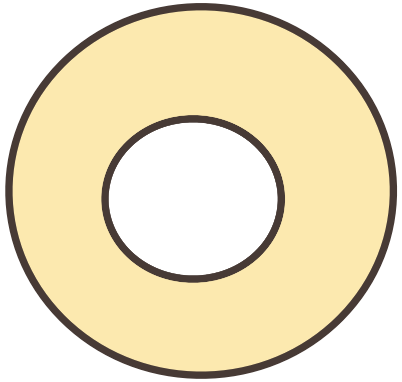
Overview

- Fundamental concepts
  - Topological space
    - Metric space topology
  - Continuous maps
  - Homeomorphisms and homotopies
  - Manifolds
    - General case, and surfaces
  - Functions on manifolds



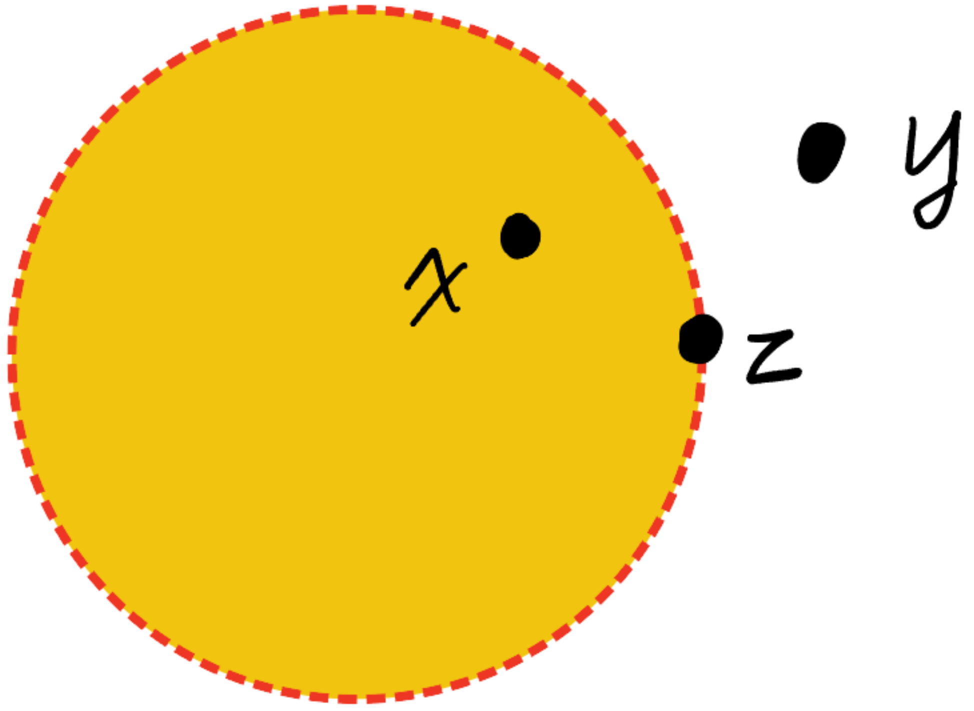


- How to rigorously describe these **continuous** transformations?

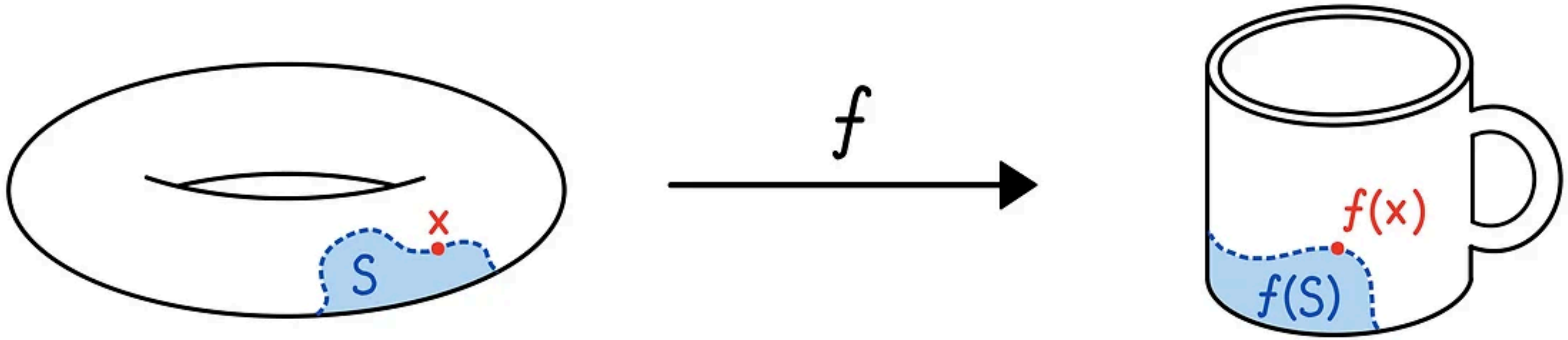
Set theory and beyond

- Given a disk D (without boundary)
  - $x \in D$
  - $y \notin D$
  - $z \notin D$ but D **contacts** z



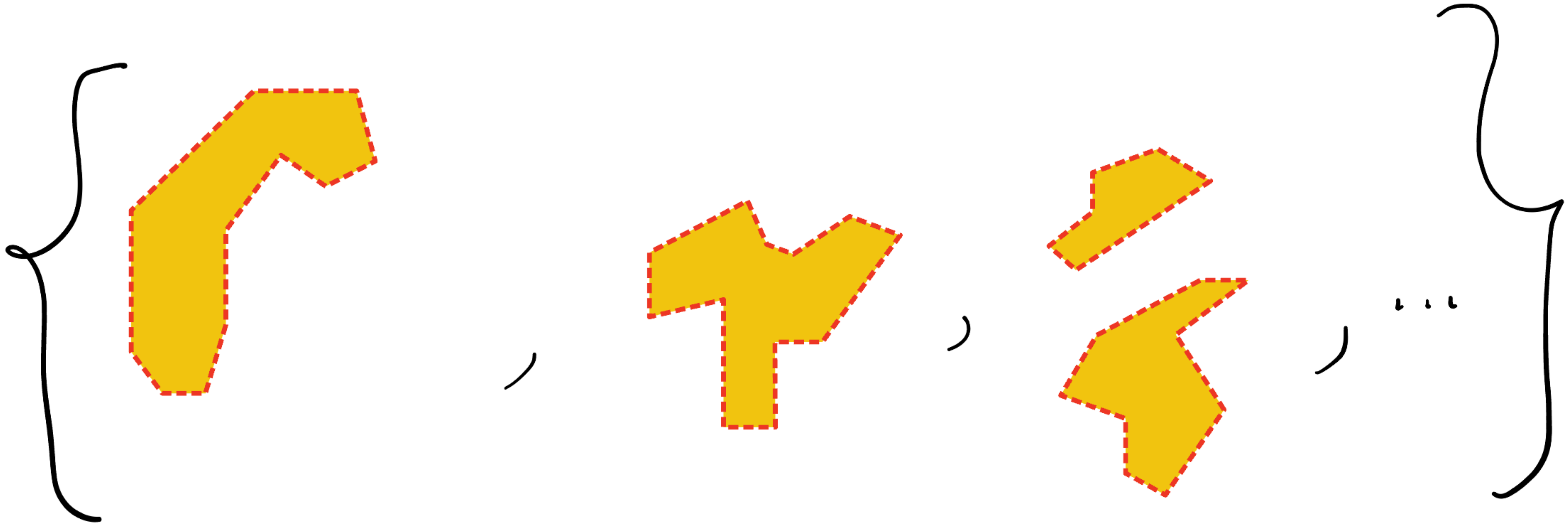
Why do we care?

- We want to rigorously define "continuous transformation"
  - If S "contacts" x, under a continuous transformation, we want that $f(S)$ "contacts" $f(x)$



From https://wgyory.wixsite.com/toolatetopologize/post/post-1

Topology



Topological space

Definition 1.1 (Topological space) *A* topological space *is a set* X *endowed with a* topological structure *(a* topology*)* $\mathcal{T}$ *such that the following conditions are satisfied:*

1. *Both the empty set and* X *are elements of* $\mathcal{T}$.
2. *Any union of arbitrarily many elements of* $\mathcal{T}$ *is an element of* $\mathcal{T}$.
3. *Any intersection of finitely many elements of* $\mathcal{T}$ *is an element of* $\mathcal{T}$.

- $\mathscr{T}$ is a system of subsets of X. It is called a topology on X .
- Examples:
  - Trivial topology $\{\emptyset, X\}$
  - Discrete topology $2^X =$ all subsets of X
  - **Metric space topology**

Open / Closed sets

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  - i.e., there exists A such that $B = \mathrm{X} \setminus A$
- Intuitively, given a set (space) X, defining open sets ($\mathscr{T}$) decides its topology.
  - Different topologies can be defined on the same space X

Connectivity

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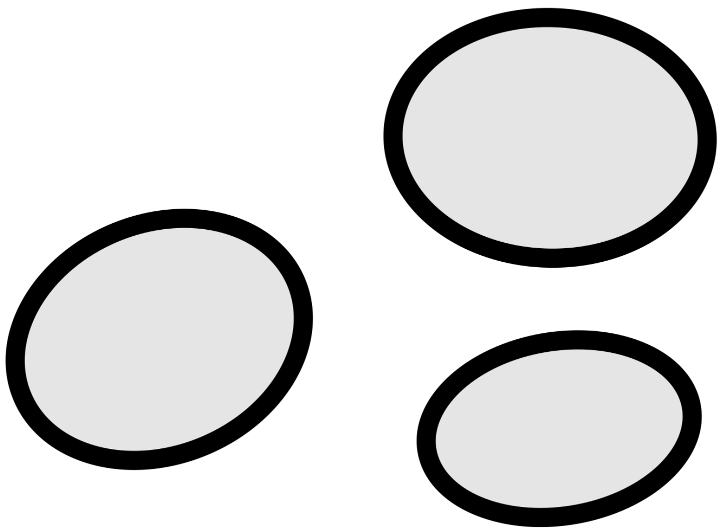

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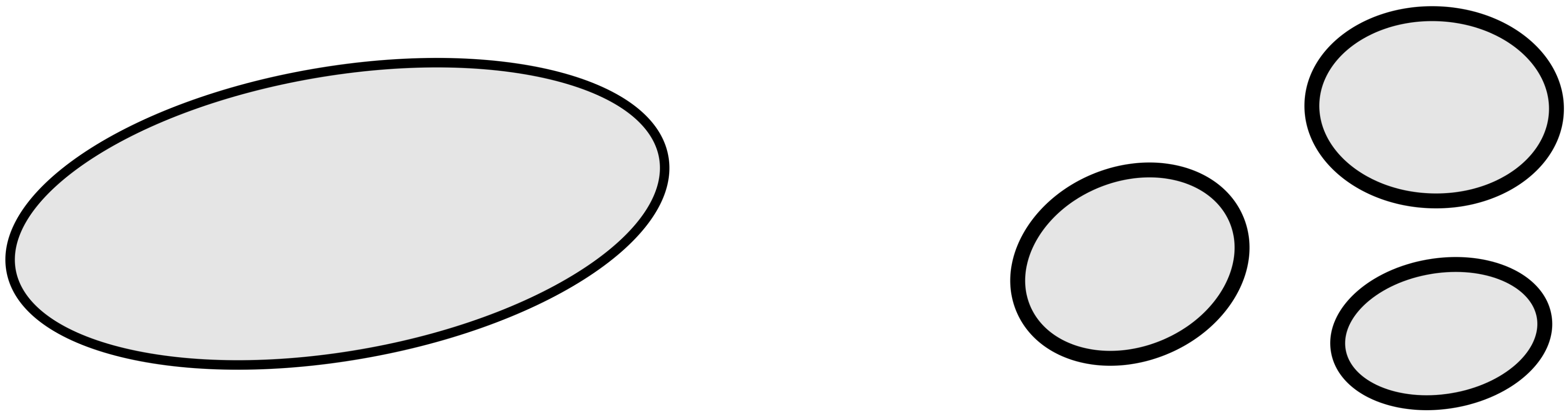

Compactness

- This generalizes the notion of **closed** and **bounded** sets in Euclidean space

- Open cover: $\mathscr{U} = \{U_\alpha\}_{\alpha\in A}$ is an open cover for $(X, \mathscr{T})$ if $U_\alpha \in \mathscr{T}$ and $X = \cup_{\alpha\in A} U_\alpha$
- $(X, \mathscr{T})$ is called compact if for any open cover $\mathscr{U} = \{U_\alpha\}_{\alpha\in A}$ there exists a finite subcover, i.e., a finite set $A' \subseteq A$ such that $X = \cup_{\alpha\in A'} U_\alpha$

- These sound too abstract! Let's use something we are familiar with, the Euclidean space, as an example
  - A set $A \subset \mathbb{R}^d$ is open if for any point $x \in A$, there exists an open ball $B_o(x, r) \subset A$.
  - Is the collection of open sets in Euclidean space a topology?
    - $\varnothing$ and $\mathbb{R}^d$ are open
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Metric space

Definition 2 (Metric space)**.** *A* metric space *is a pair* (X, d) *where* X *is a set and* d *is a distance function* $\mathsf{d} : \mathsf{X} \times \mathsf{X} \to \mathbb{R}$ *satisfying the following properties:*

- $\mathsf{d}(p, q) = 0$ *if and only if* $p = q$
- $\mathsf{d}(p, q) = \mathsf{d}(q, p), \forall p, q \in \mathsf{X}$*;*
- $\mathsf{d}(p, q) \leq \mathsf{d}(p, r) + \mathsf{d}(r, q), \forall p, q, r \in \mathsf{X}$.

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- Examples:
  - $(\mathbb{R}^k, \|\cdot\|_2)$ k-dimensional Euclidean space, equipped with the standard Euclidean distance $d(p, q) = \|p - q\|_2$
  - "Curved" space (manifolds), equipped with geodesic distance
    - e.g, the surface of earth.
  - Space can also be discrete, as very often in data analysis
    - $(P, \ d)$: a set of points with pairwise distance (or similarity) given.
    - or graphs, equipped with shortest path metric.

Metric space topology

- Open ball:
  - $B_o(c,\ r) = \{x \in X \mid d(c, x) < r\}$

Definition 3 (Metric space topology). *Given a metric space* X, *all metric balls* $\{B_o(c, r) \mid c \in \mathbb{T}$ *and* $0 < r \leq \infty\}$ *and their union constituting the open sets define a topology on* X.

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- The set of metric balls is called a *basis* for this topology on X
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- In general, when we refer to a common metric space, say Euclidean space, we refer to this metric space topology induced by standard metric.

Metric space topology on $\mathbb{R}$

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- Each open ball is an open interval $(c - r, c + r)$

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Exercise: why?

Closure, interior, boundary

Closure, interior, boundary

- Recall a set is closed if its complement is open
- Given a topological space $(\mathsf{X}, \mathscr{T})$ and a subset $A \subseteq \mathsf{X}$:
  - the *closure* of A, denoted by $Cl(A)$, is the smallest closed set containing A.
  - its *interior* $\mathrm{Int}(A)$ is the union of all open subsets of A.
  - the *boundary* of A is $\mathrm{bnd}(A) = A \setminus Int(A)$

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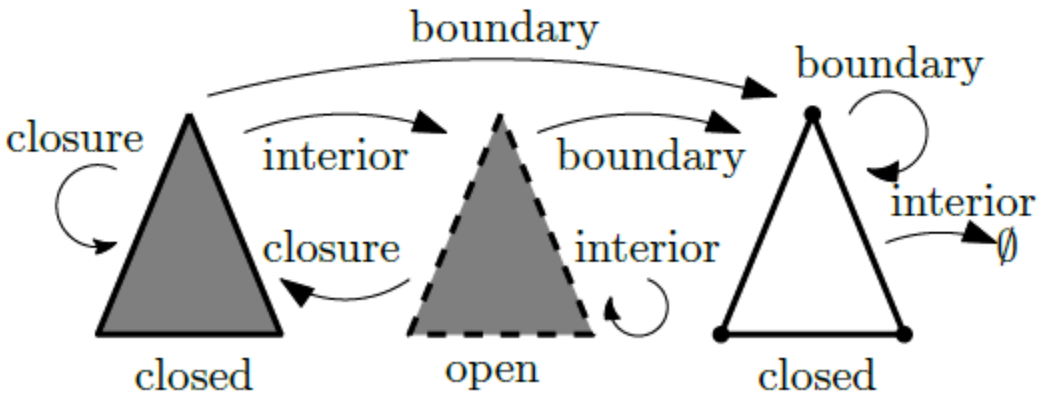

Examples in $\mathbb{R}$

- Let $A = [1,2)$
  - $Cl(A) = [1,2]$
  - $Int(A) = (1,2)$
  - $Bnd(A) = \{1,2\}$

Subspace topology

- A topological space $(\mathsf{X}, \mathscr{T})$, say the Euclidean space
- Given a subset $Y \subseteq \mathsf{X}$, the subspace topology $\left(Y, \mathscr{T}_Y\right)$, (inherited from $(\mathsf{X}, \mathscr{T})$), is such that $\mathscr{T}_Y$ consists of intersection between open sets in $\mathscr{T}$ and Y.

- Common subspaces of Euclidean space
  - Euclidean d-ball: $\mathbb{B}^d = \left\{x \in \mathbb{R}^d \mid \|x\| \leq 1\right\}$
  - Open Euclidean d-ball: $\mathbb{B}_o^d = \left\{x \in \mathbb{R}^d \mid \|x\| < 1\right\}$
  - Euclidean d-sphere: $\mathbb{S}^d = \left\{x \in \mathbb{R}^{d+1} \mid \|x\| = 1\right\}$
  - Euclidean half-space: $\mathbb{H}^d = \left\{x \in \mathbb{R}^d \mid x_d \geq 0\right\}$

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- Example: $X = \mathbb{R}$ and $Y = [1,2]$. Then, $(1.5,2] = (1.5,3) \cap [1,2]$ is an open set in subspace topology.

Check-in: Where are we?

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How we mathematically talk about space of interest

Now we need ways to connect different spaces!

Continuous function

Continuous function

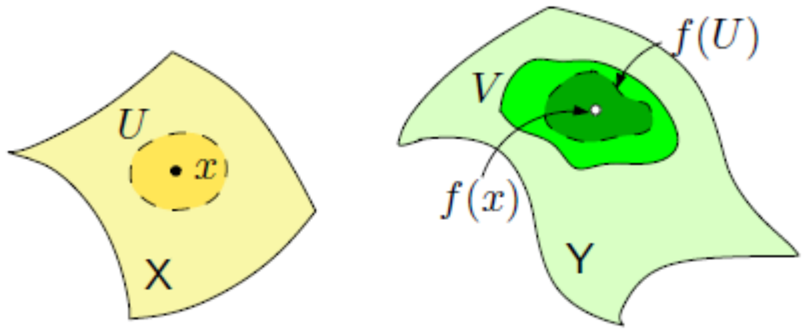
- Recall the simple case $f: R \to R$
  - f is continuous at $x \in \mathbb{R}$ if for any $\epsilon > 0$, there exists $\delta > 0$ such that for any $y \in (x - \delta, x + \delta)$, $f(y) \in (f(x) - \epsilon, f(x) + \epsilon)$

- Equivalently, for any open neighborhood $B_o(f(x), \epsilon)$ of $f(x)$, there exists an open neighborhood $B_0(x, \delta)$ of x such that $f(B_o(x, \delta)) \subset B_o(f(x), \epsilon)$

Continuous function

Definition 4 (Continuous function) *A* neighborhood *of a point $x \in \mathsf{X}$ is simply a subset of X that contains some open set U such that $x \in U$. A function $f : \mathsf{X} \to \mathsf{Y}$ is* continuous at $x \in \mathsf{X}$ *if for any neighborhood V of $f(x)$, there is a neighborhood U of x such that $f(U) \subseteq V$. See the right figure for an illustration. Function f is* continuous *if it is continuous at all points in X.*

Equivalently, a function $f : \mathsf{X} \to \mathsf{Y}$ is continuous *if for any open set V in Y, its preimage $f^{-1}(V)$ is also open.*



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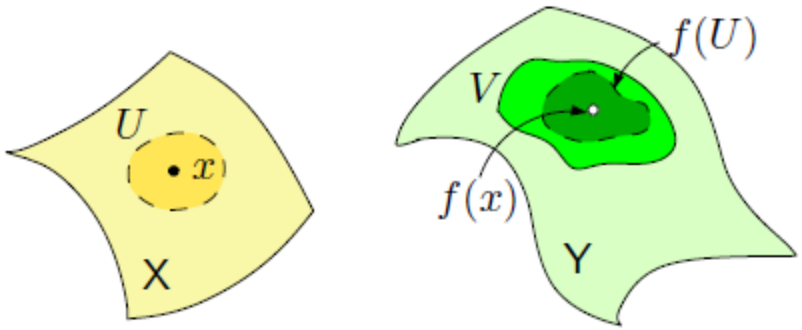

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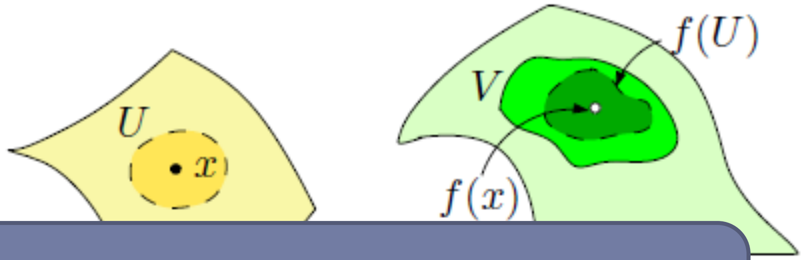

The Preimage of an open set is open

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Describe relations of spaces

Homeomorphism = homoios + morphē = Similar shapes

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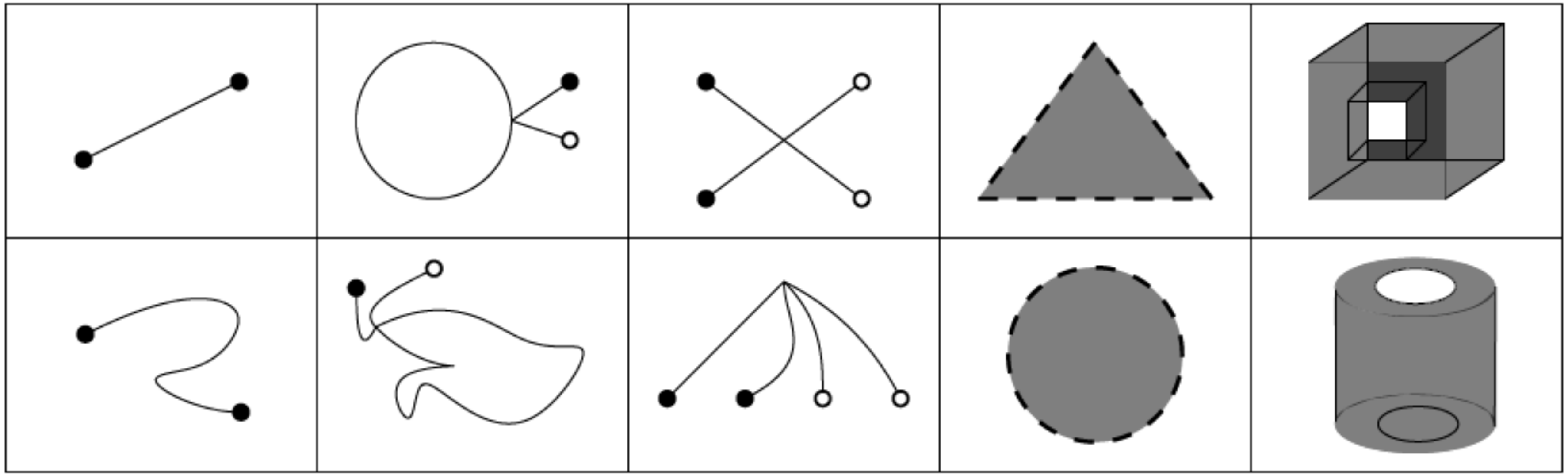
- Essentially, two spaces are "equivalent" in terms of open-set topology
  - Homeomorphic spaces are called *topologically equivalent*
    - Note that equivalent relations are transitive.
  - Layman's terms: two spaces are homeomorphic if one can continuously deform (stretch, compress) into the other without ever breaking or stitching them
    - Not always true

Examples

Examples



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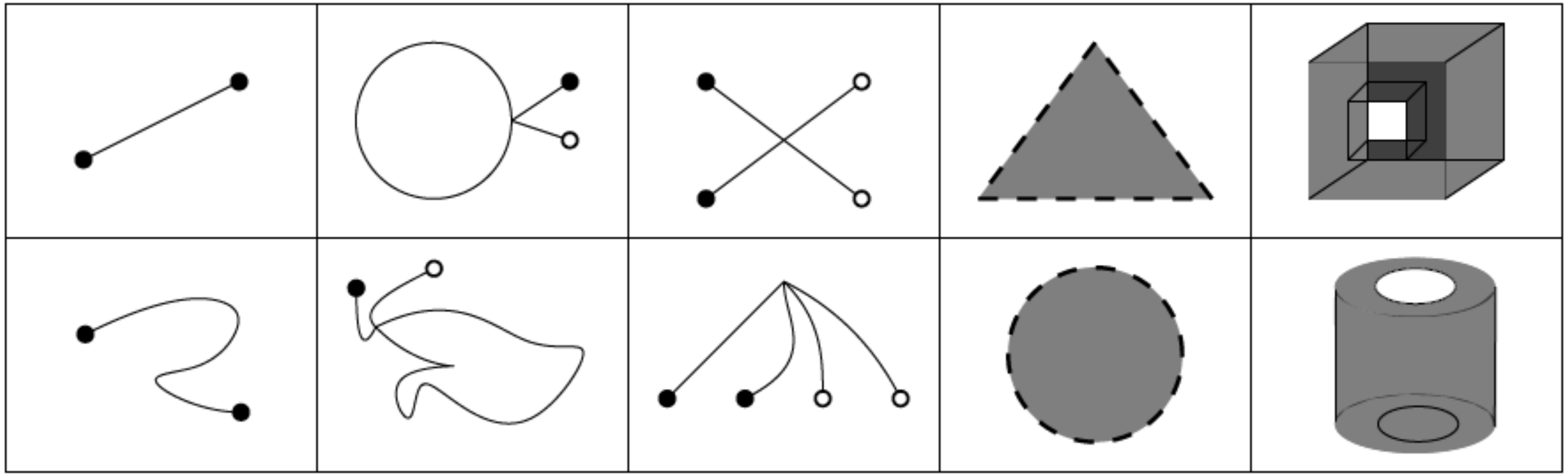

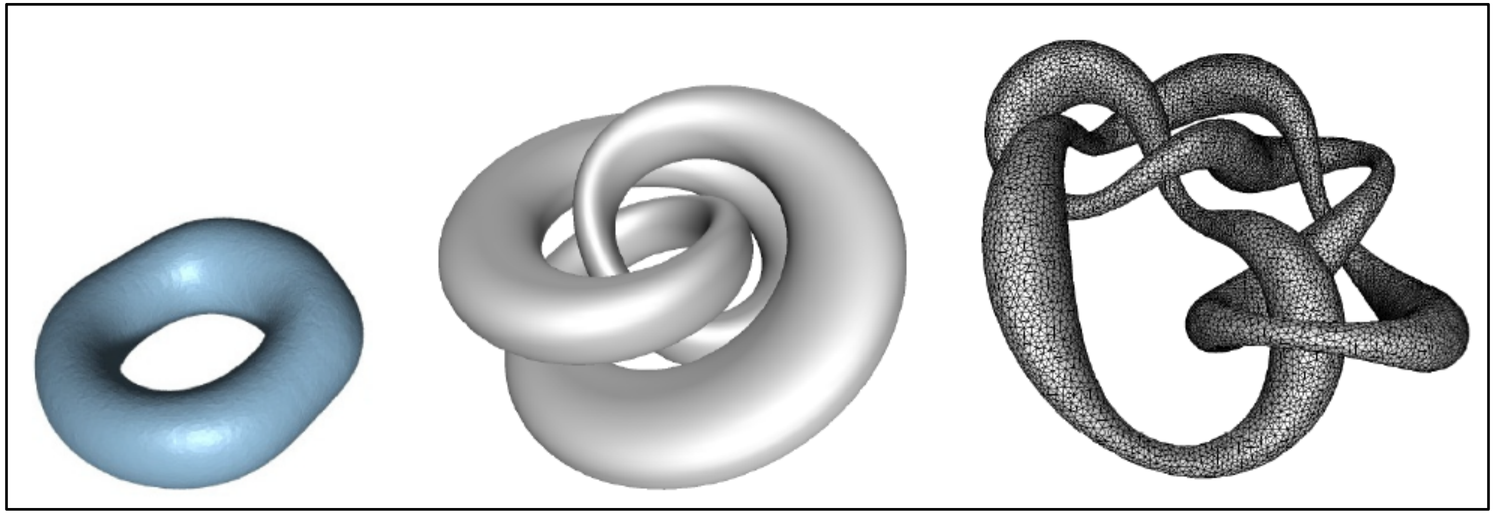

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- A trick: remove one point and check connected components
  - Y and I are not homeomorphic; X and Y are not homeomorphic
  - $\mathbb{R}$ and $\mathbb{R}^2$ are not homeomorphic
  - What about $\mathbb{R}^2$ and $\mathbb{R}^3$?
- In general, hard to decide whether two spaces are homeomorphic or not!

A weaker notion: Homotopy equivalent

- When X, Y are homeomorphic, there exists continuous functions $f : X \to Y, g : Y \to X$ such that $f \circ g = Id_Y$ and $g \circ f = Id_X$

- Can we have a weaker notion of $=$? How about we consider continuous transition from $f \circ g$ to Id_Y?

A weaker notion: Homotopy equivalent

Definition 6 (Homotopy) *First, two* $f, g : \mathsf{X} \to \mathsf{Y}$ *are* homotopic *if there is a continuous map* $H : \mathsf{X} \times [0,1] \to \mathsf{Y}$ *such that* $H_0 = f$ *and* $H_1 = g$*. This map* H *is called a* homotopy *connecting* f *and* g.

Definition 7 (Homotopy equivalence) *Two spaces* X *and* Y *are homotopy equivalent if there is a continuous mapping* $f : X \to Y$ *and* $g : Y \to X$ *such that* $f \circ g$ *is homotopic to identity in* Y *and* $g \circ f$ *is homotopic to identity in* X.

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  - Two homeomorphic spaces X and Y are also homotopy equivalent. But the inverse may not hold.

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- Homotopy equivalent relation is transitive.

- In general, hard to establish homotopy equivalent relation as well
- One useful special case: Deformation retraction

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We say that $A \subseteq X$ is a deformation retract of X *if there is a retraction r that is homotopic to the identity map in X. This retraction map is called a* deformation retraction.

Equivalently, a continuous map $R : X \times [0,1] \to X$ is a deformation retraction of X onto A *if for every $x \in X$ and $a \in A$, $R(x,0) = x$; $R(x,1) \in A$ and $R(a,1) = a$.*

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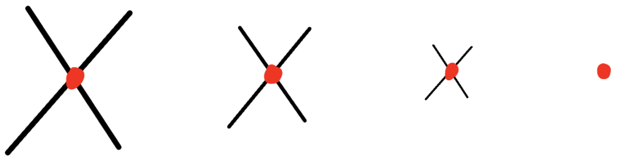
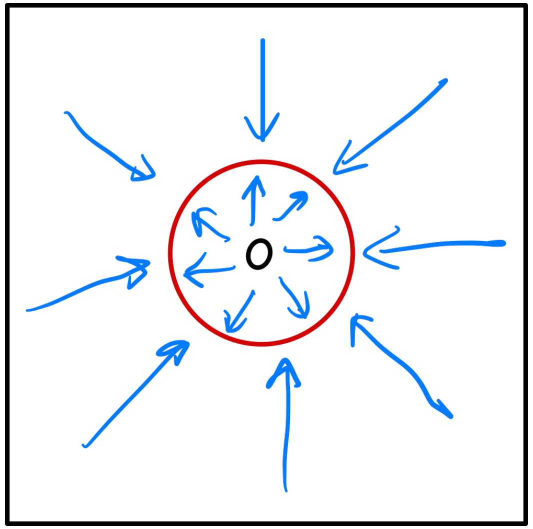
- Theorem:
  - If Y is a deformation retract of X, then X and Y are homotopy equivalent.

Examples

- X and Y are homotopy equivalent but not homeomorphic



- A disk and a point
- A tree and a point
- A punctured plane and a circle



$$R : [0,1] \times \mathbb{R}^2 \backslash 0 \to \mathbb{R}^2 \backslash 0$$

$$R(t, x) = (1-t)x + t\frac{x}{\|x\|}$$

Examples

- A punctured torus $\approx$?

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Examples

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Both homeomorphism and homotopy equivalence can be hard to detect, and not computationally friendly in general. Later we will focus on homology, which is much easier to compute.

Check-in: Where are we?

- Fundamental concepts
  - Topological space
    - Metric space topology
  - Continuous maps
  - Homeomorphisms and homotopies
  - Manifolds
    - General case, and surfaces
  - Functions on manifolds

How we mathematically talk about space of interest

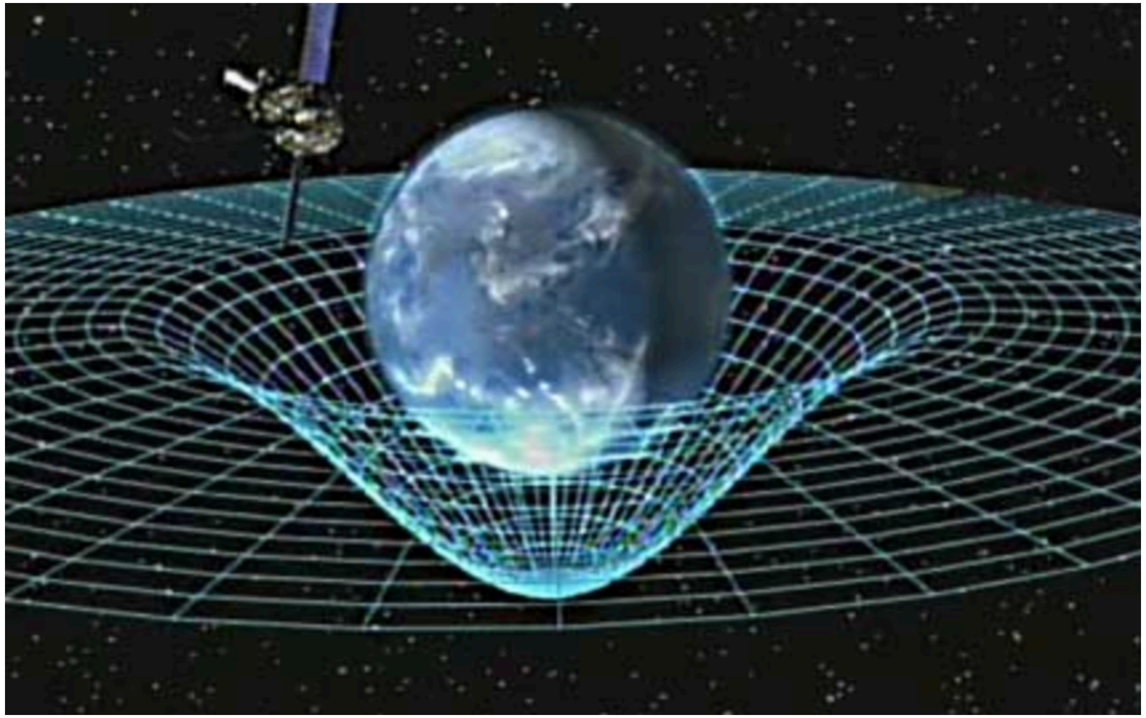
Now we need ways to connect different spaces!

Describe relations of spaces

A generalization of Euclidean space; a special type of topological space

Why manifolds?

- We like Euclidean spaces. Why manifolds?



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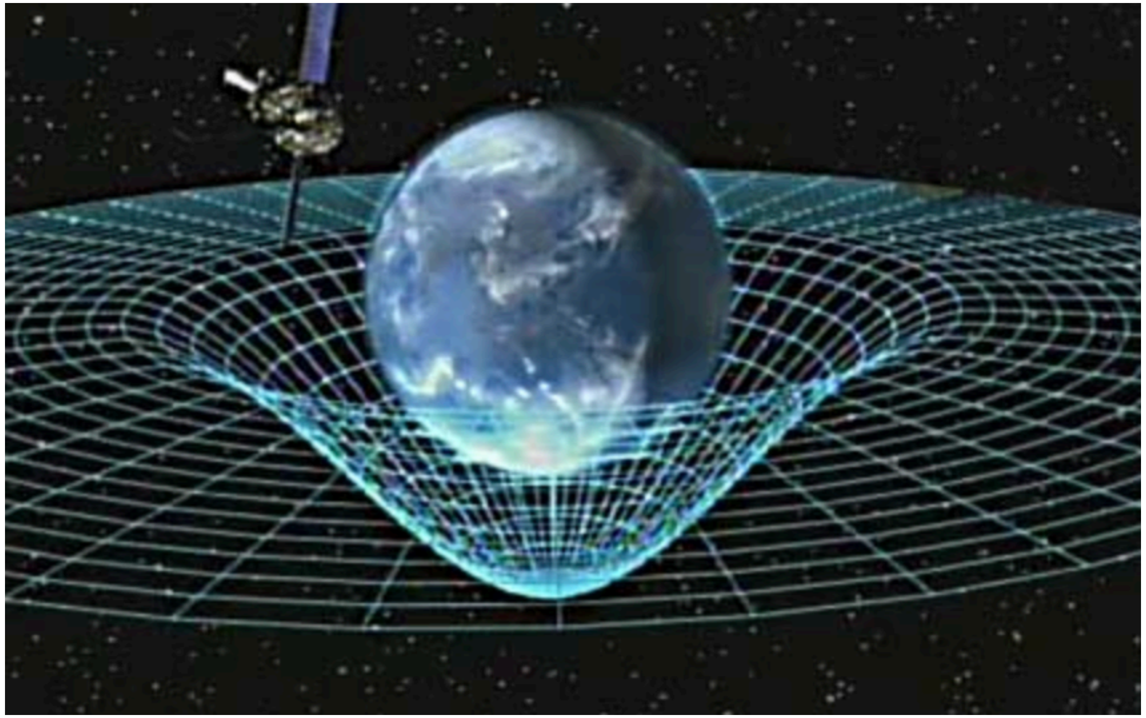
  - We live in non-Euclidean space



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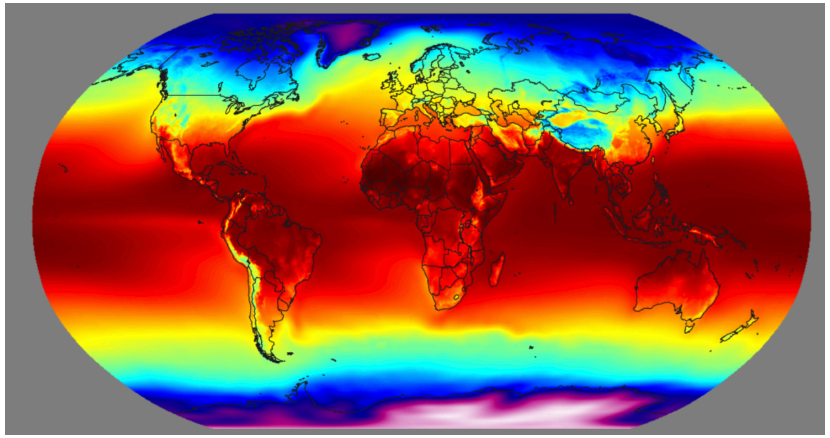

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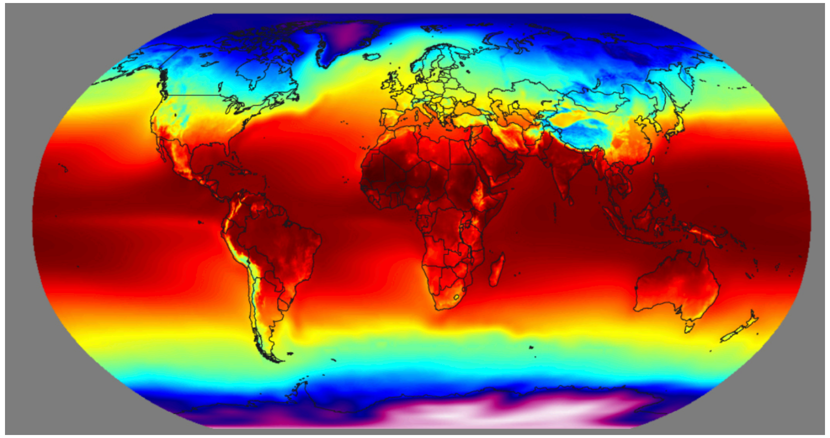

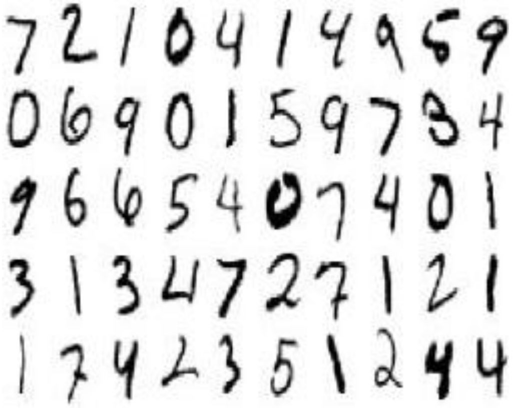

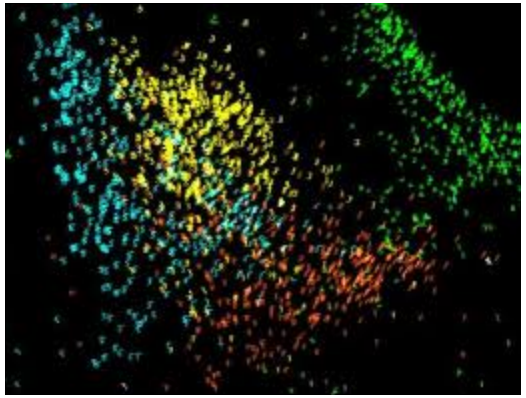

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  - The intrinsic space may not be a linear subspace of the ambient space
    - e.g, the surface of a bunny in $\mathbb{R}^3$

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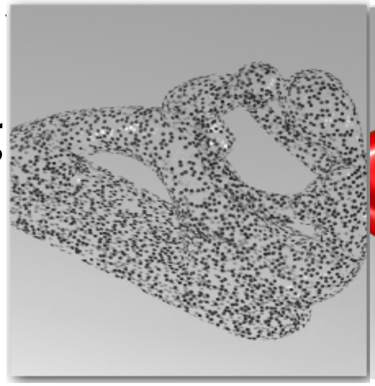
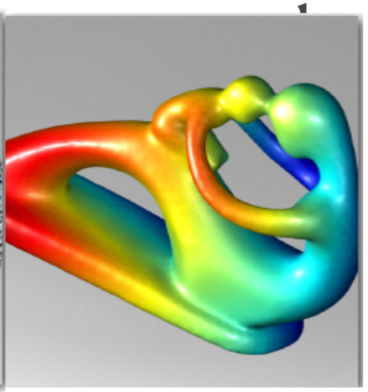
  - The   a linear subspace of the ambient space
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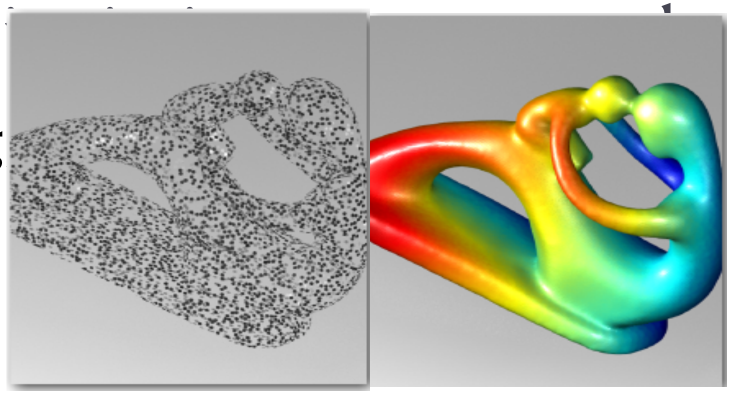

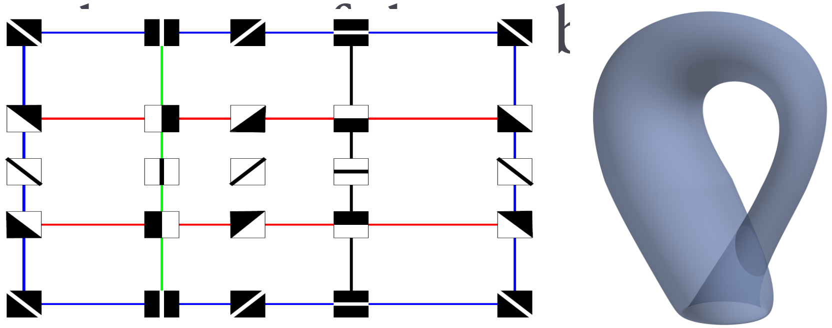

Courtesy of Carlsson et al, *On the local behavior of spaces of natural images*

What are manifolds

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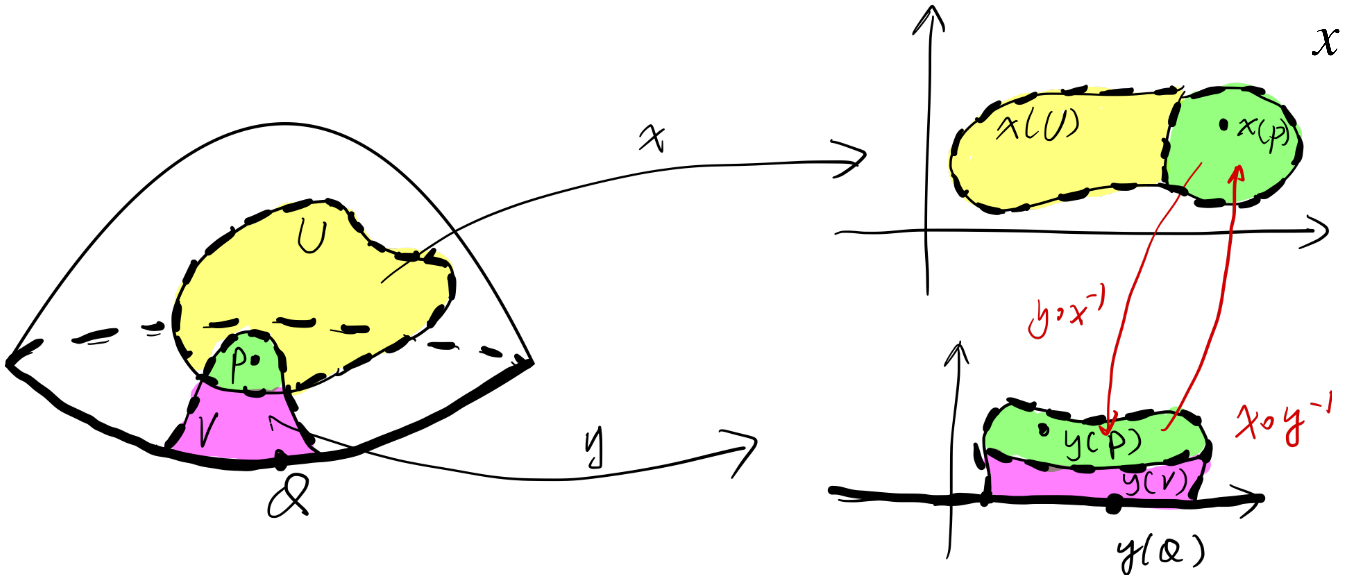

$x : U \to x(U) \subseteq \mathbb{R}^2$ is called a **coordinate chart**

$x \circ y^{-1}$ is a homeomorphism. If $x \circ y^{-1}$ is smooth, then M is called a **differentiable manifold**

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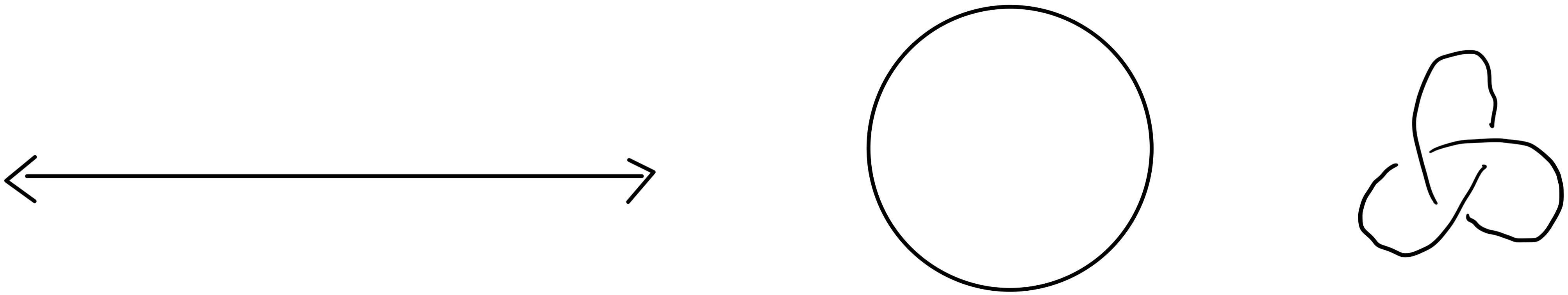
- Interior of M:
  - those points with a neighborhood homeomorphic to $\mathbb{B}_o^d$
- Otherwise, boundary of M

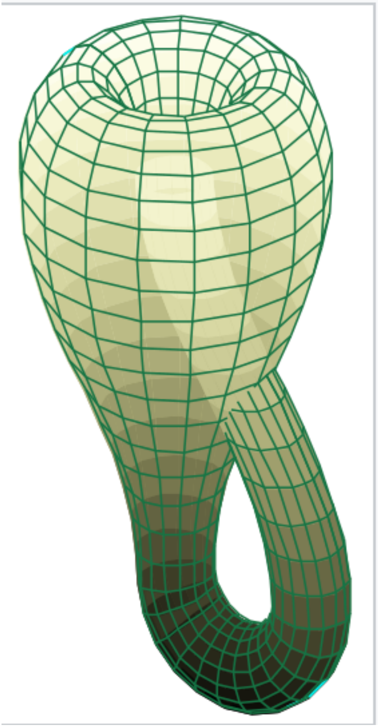
Examples

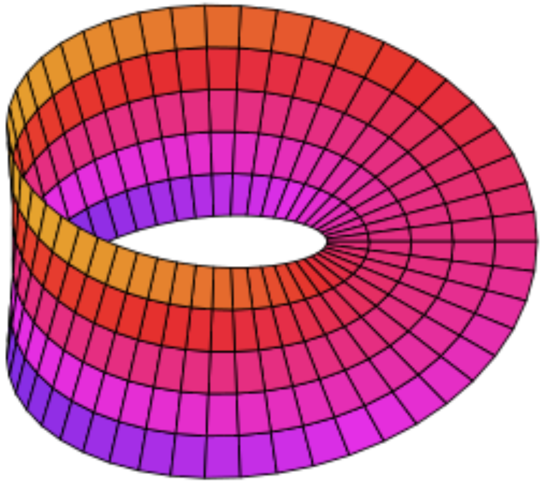
- 1-manifolds



Examples

- 1-manifolds
- 2-manifolds

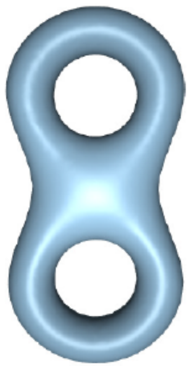
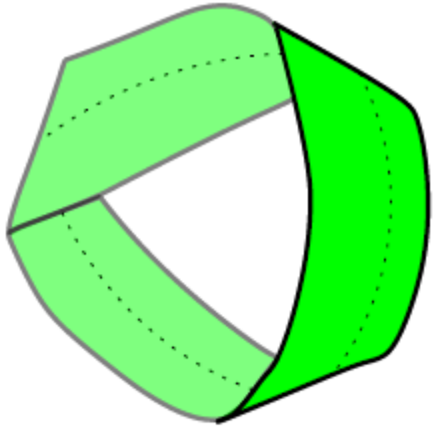




Are these manifolds?

Surfaces

- A surface is a 2-manifold
  - Locally, it looks like either an open disk, or a half-disk

- A 2-manifold M is non-orientable if
  - Starting from some point $p \in M,$ one can walk on one side of M and end up on the opposite side of M upon returning to p
- Otherwise, it is orientable.

Surfaces

- While in general it is hard to decide whether two spaces are homeomorphic or not, it turns out that we can characterize compact surfaces (without boundary) completely

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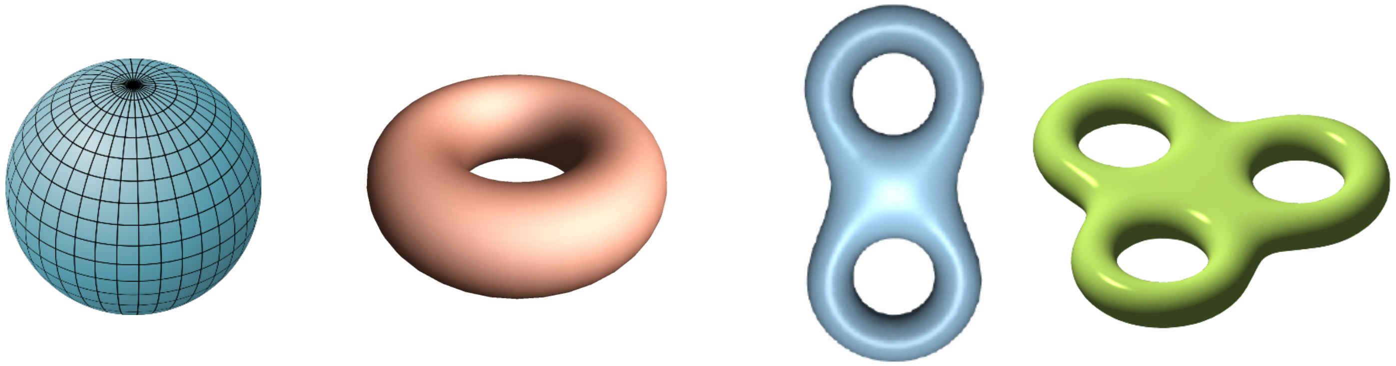

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    - Obtained by identifying antipodal points from boundary of a disk
  - Klein bottle (non-orientable)
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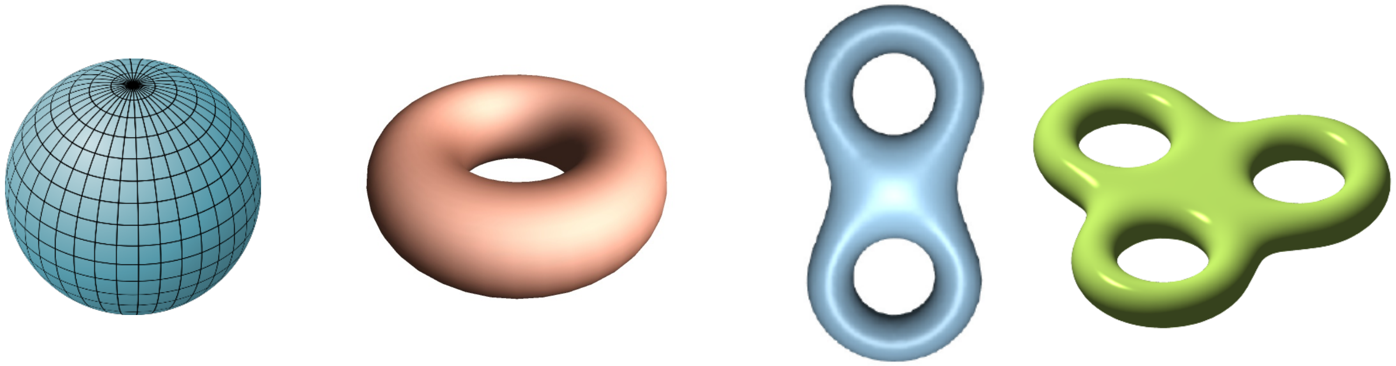

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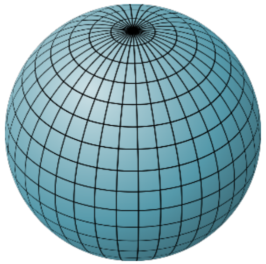
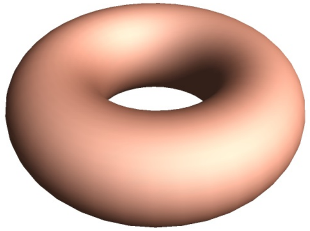
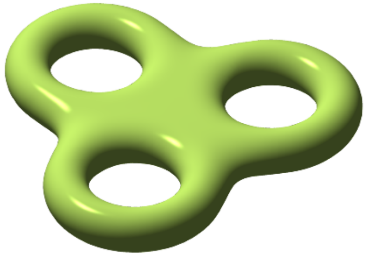
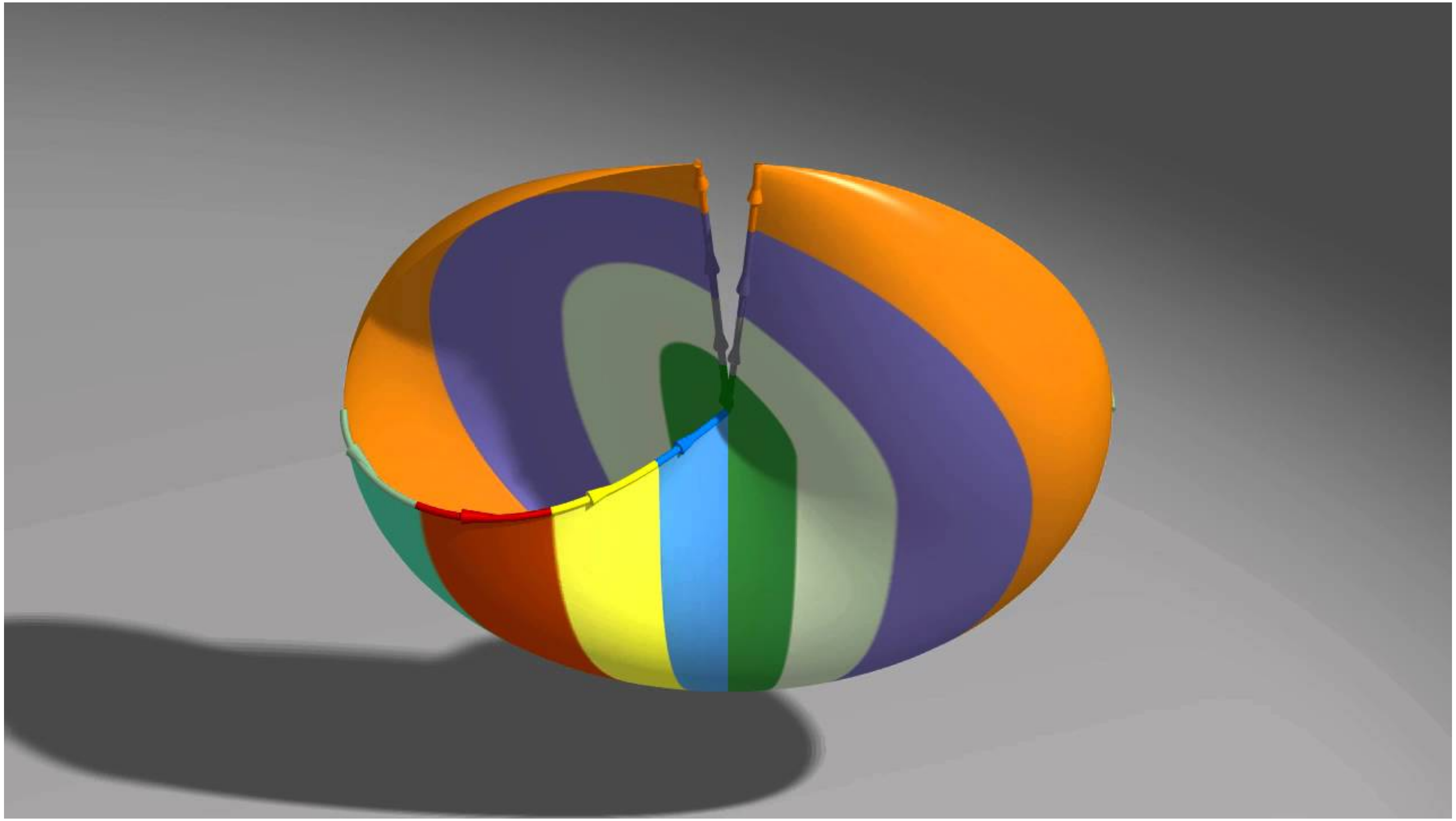






Visualization of projective plane



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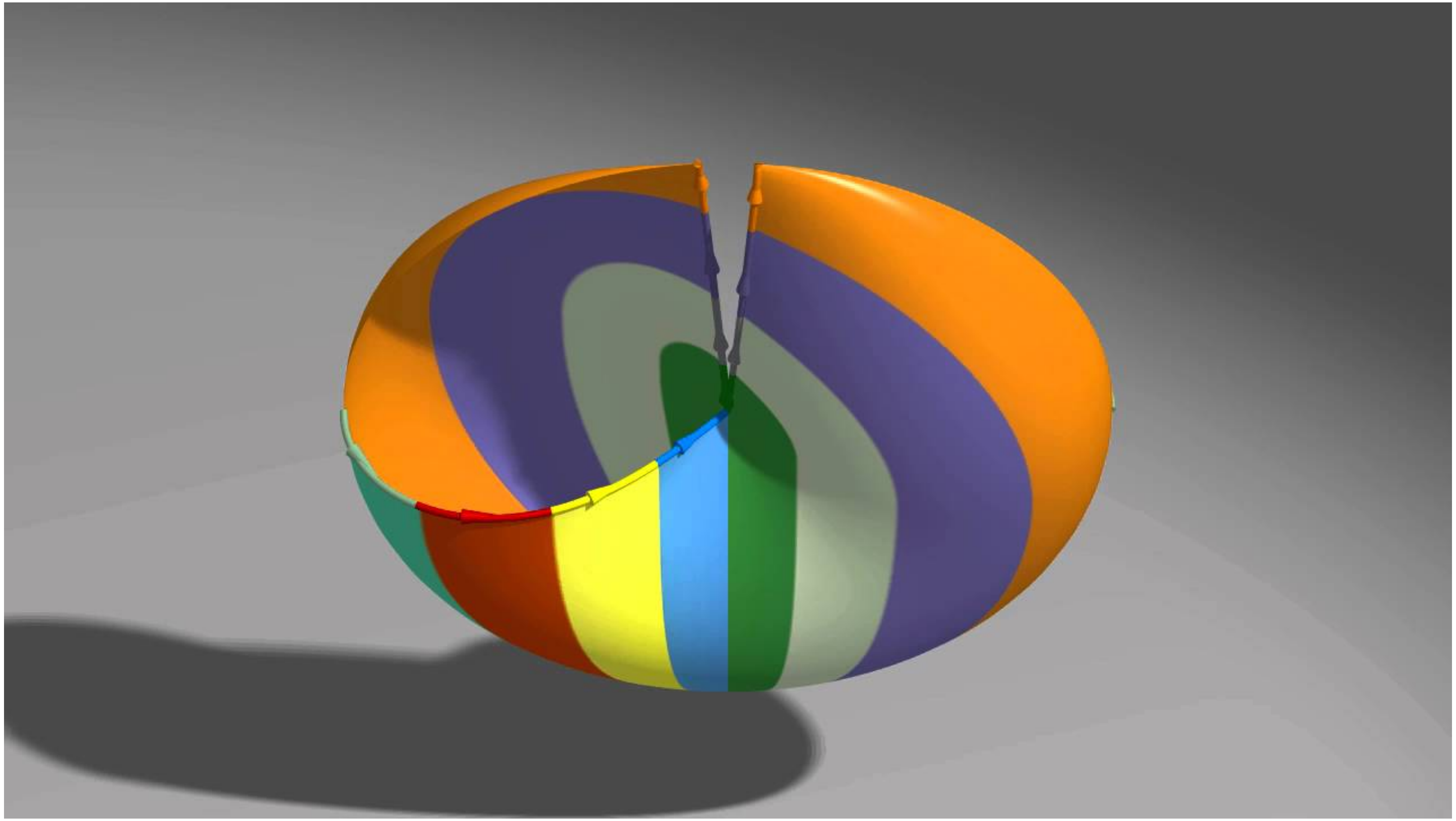
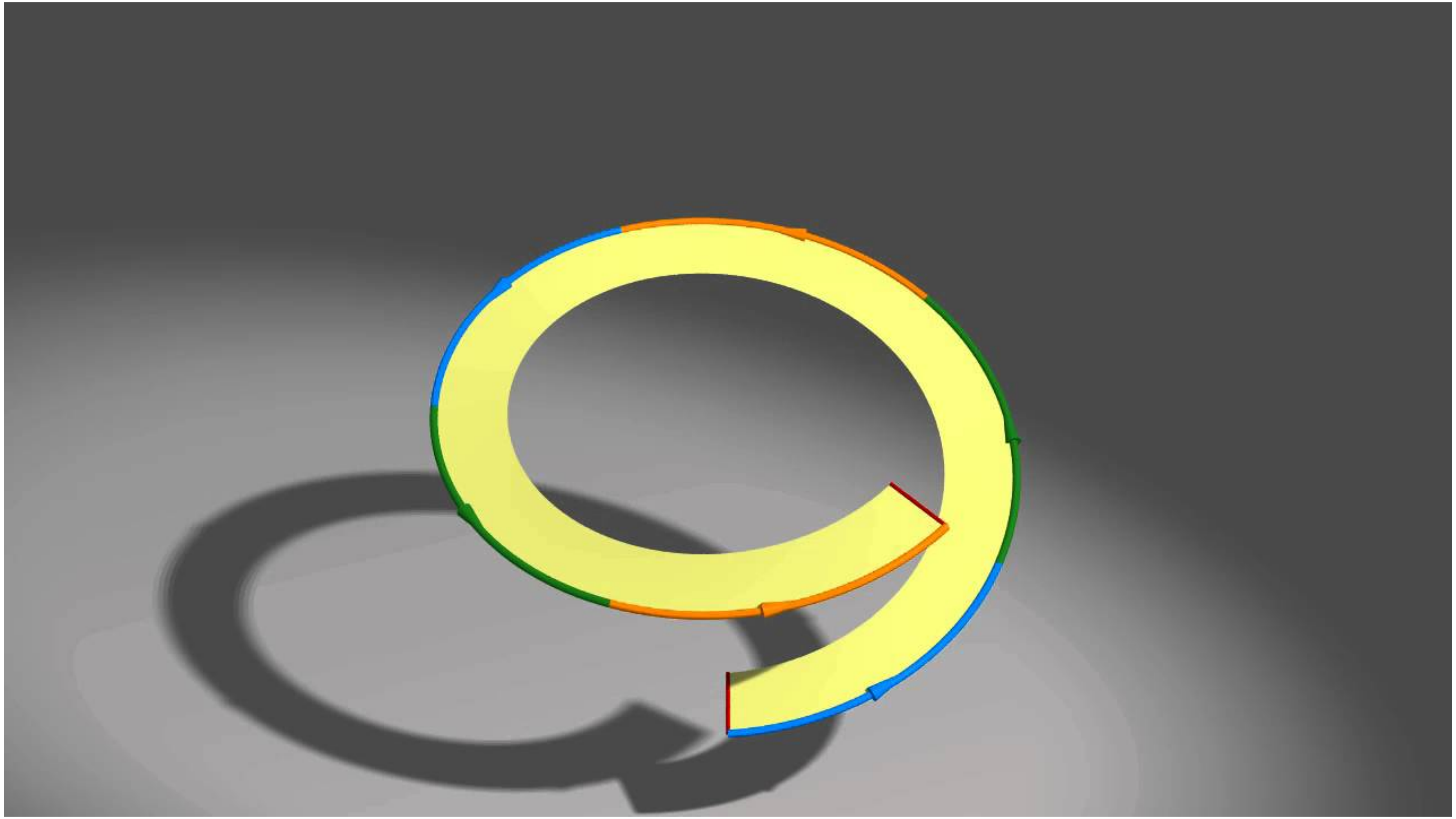


Projective plane = Mobius strip + a disk



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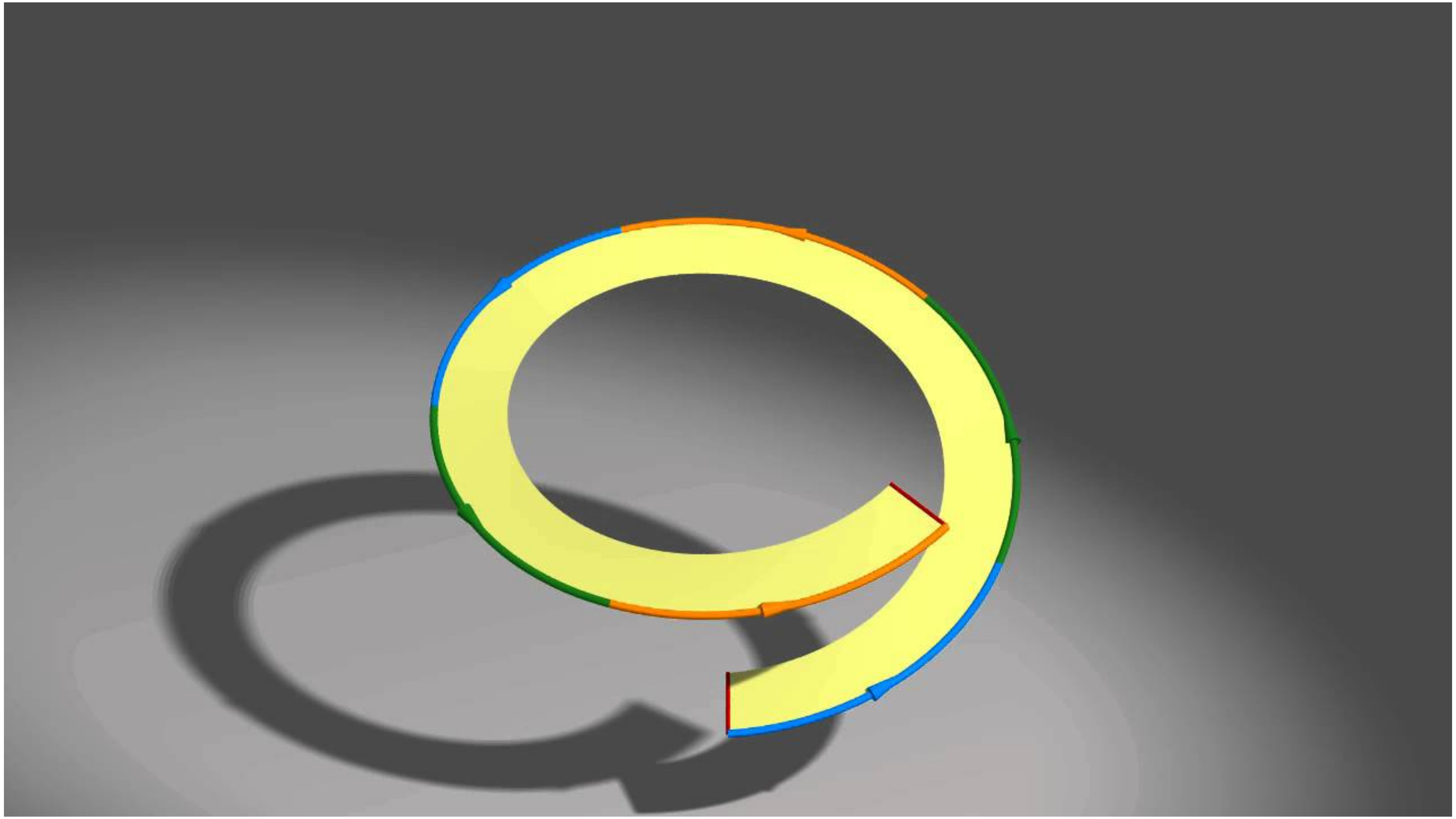
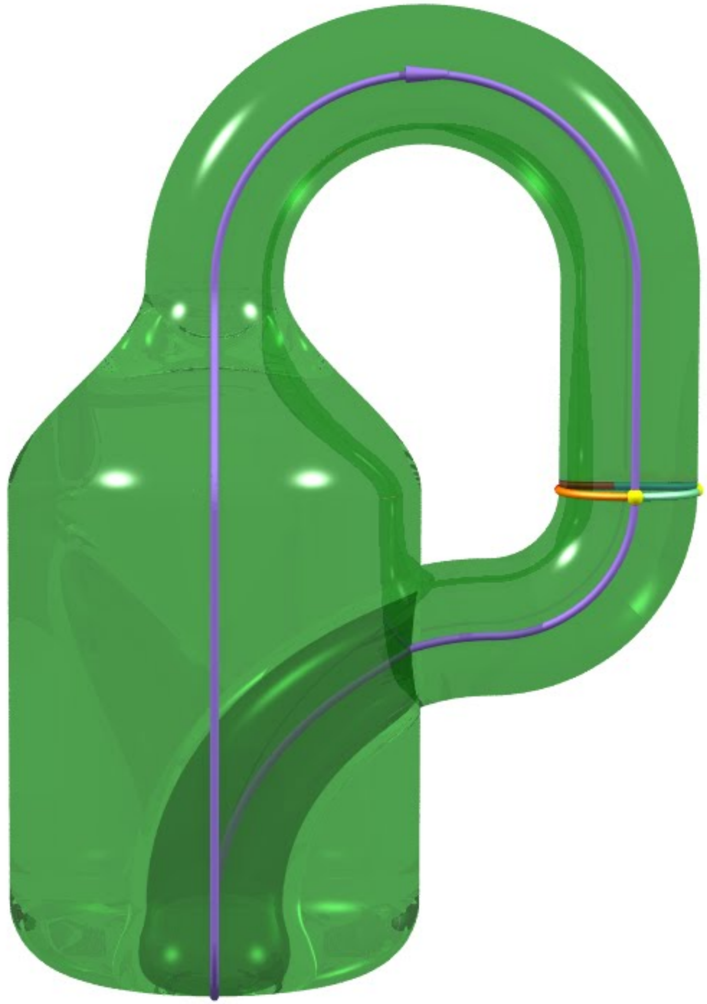


Visualization of Klein bottle



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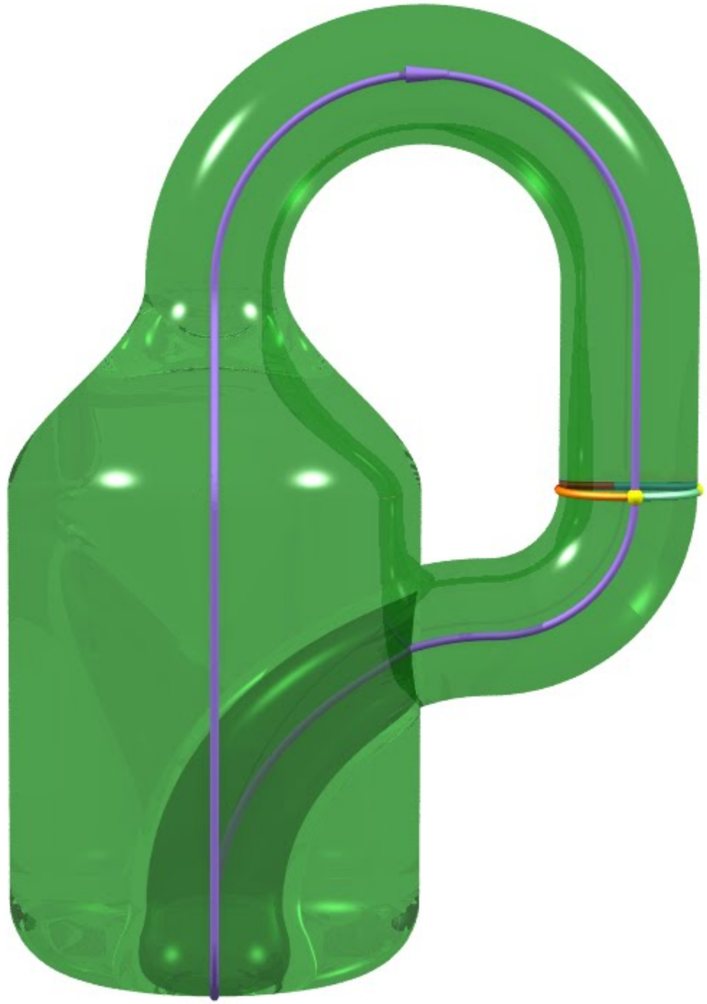
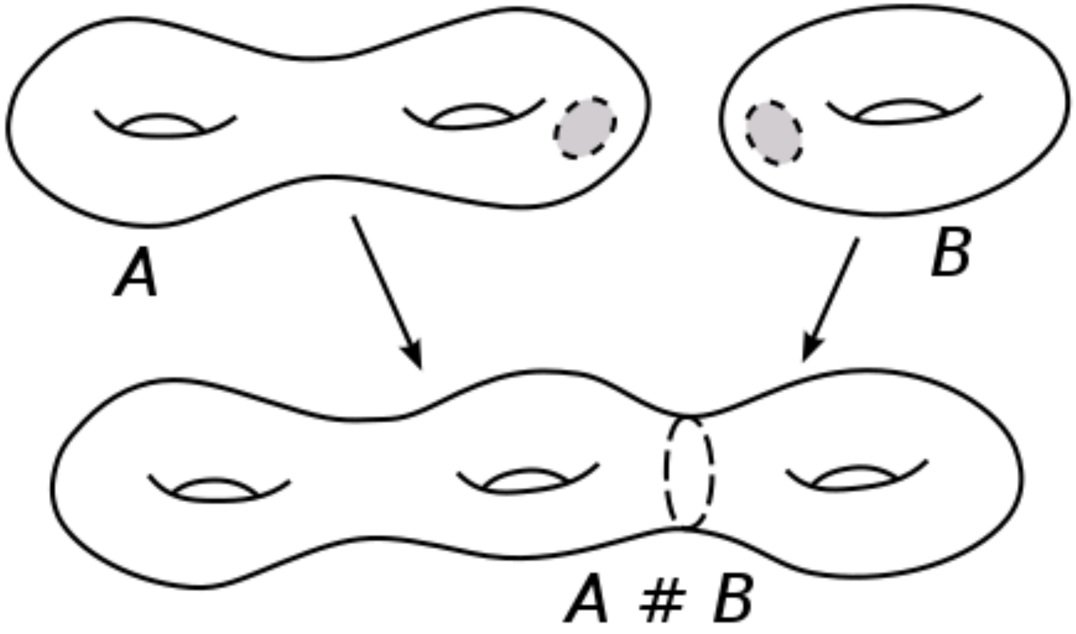


Connected sum operation

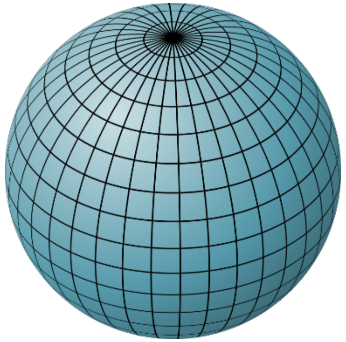
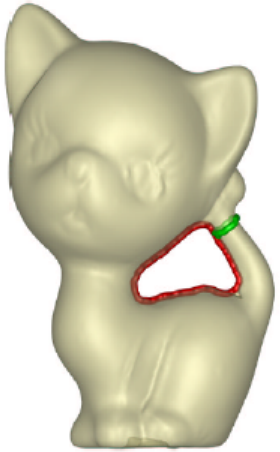
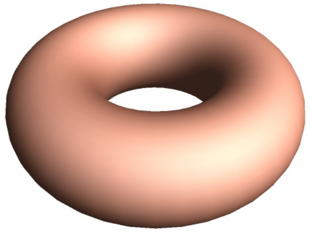
- Given two compact surface M and S, the connected sum $M\#S$ intuitively "merge" the two by cutting off a small disk (cap) from each surface, and the glue the remaining of the two surfaces along the boundary after the cutting.



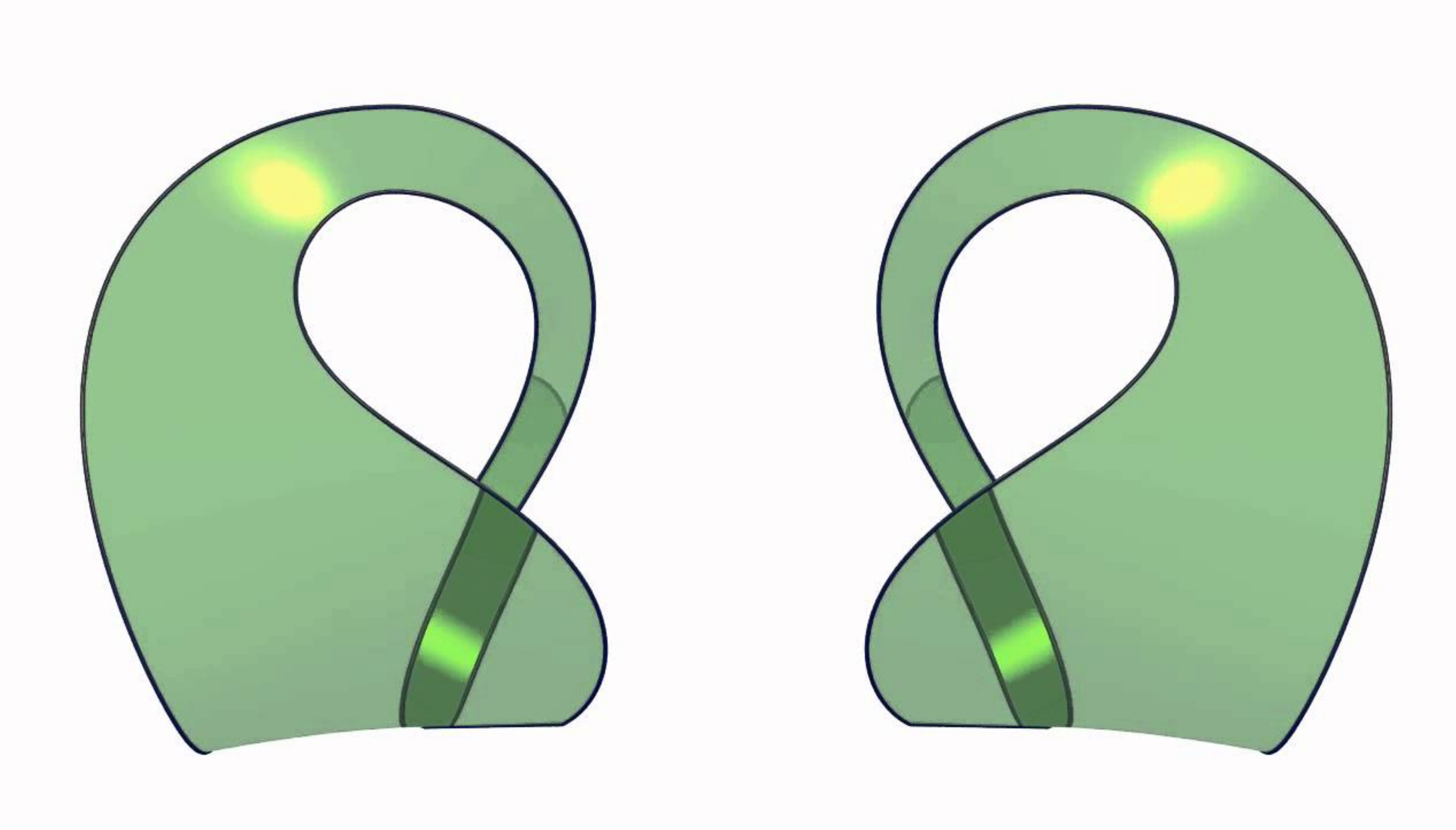
Wikipedia

Classification of compact surfaces

Theorem 2 (Classification Theorem) *The two infinite families* $\mathbb{S}$, $\mathbb{T}$, $\mathbb{T}\#\mathbb{T}$, ..., *and* $\mathbb{P}$, $\mathbb{P}\#\mathbb{P}$, ..., *exhaust the family of compact 2-manifold without boundary (upto homeomorphism). The first family of surfaces are all orientable; while the second family are all non-orientable. Furthermore, no two surfaces in these sequences are homeomorphic.*

How does $\mathbb{P}\#\mathbb{P}$ become the Klein bottle?



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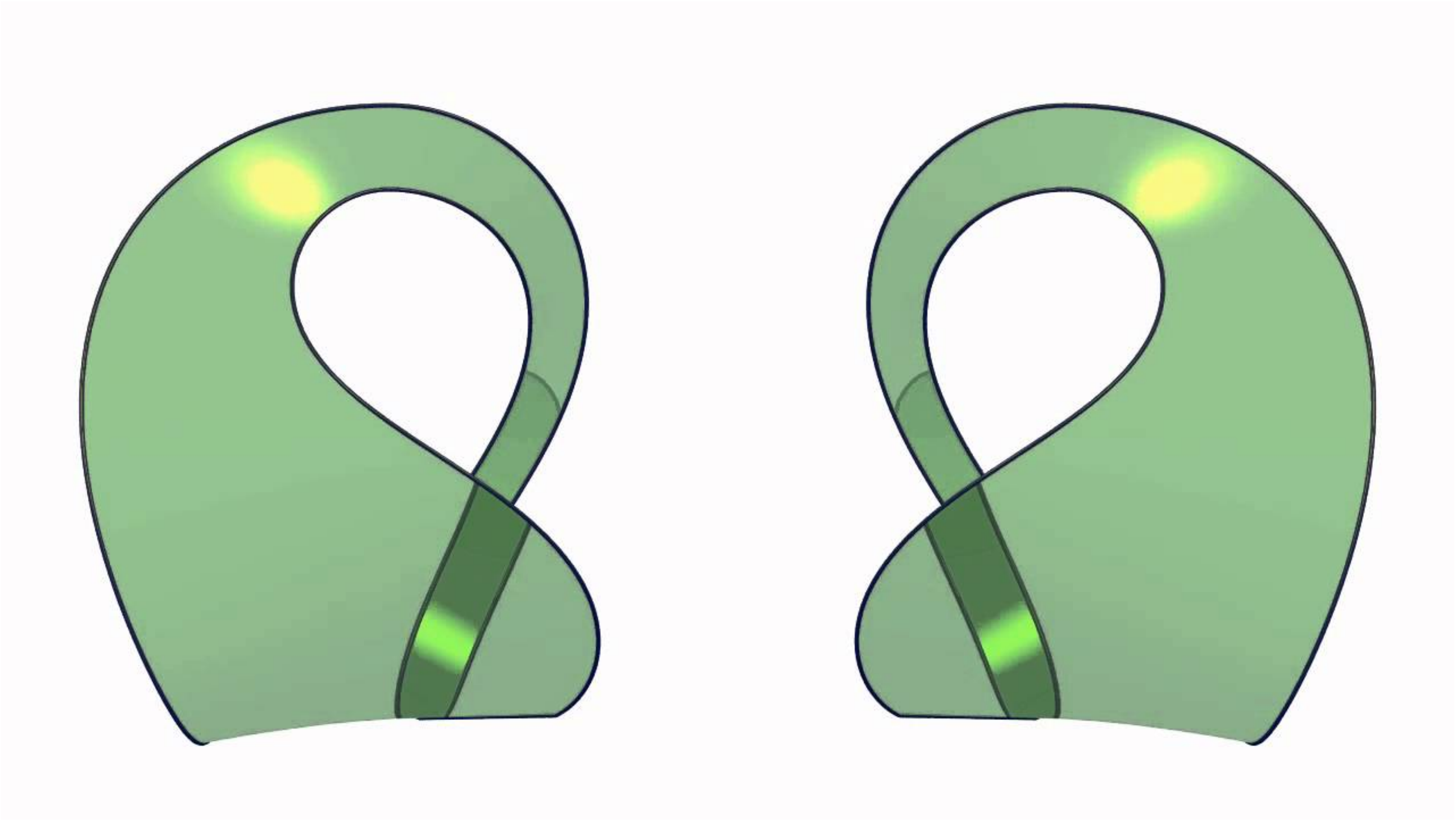

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- Intuitively
  - all orientable surfaces without boundaries can be generated by gluing handles to a sphere
- The number of $\mathbb{T}$ or $\mathbb{P}$ needed is called the genus g of the surface M
  - Sphere has genus 0, torus has genus 1, double-torus has genus 2.
- Hence the genus of a surface completely decides its topology upto homeomorphism
  - Any two compact surfaces with the same genus are homeomorphic

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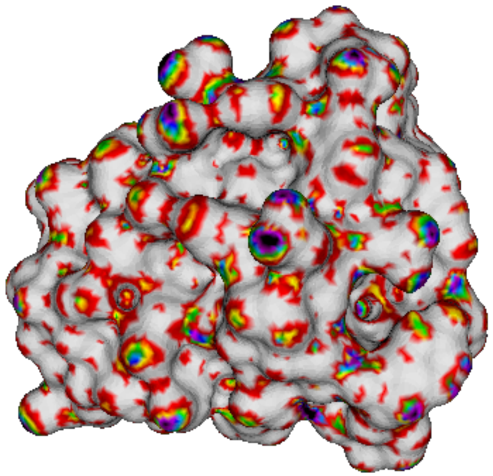
Describe relations of spaces

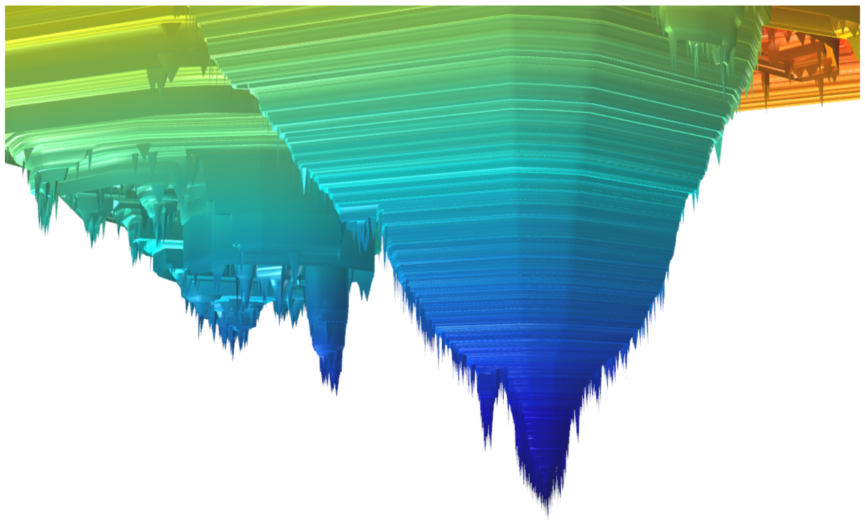
A generalization of Euclidean space

Modeling attributes on space

Functions on spaces

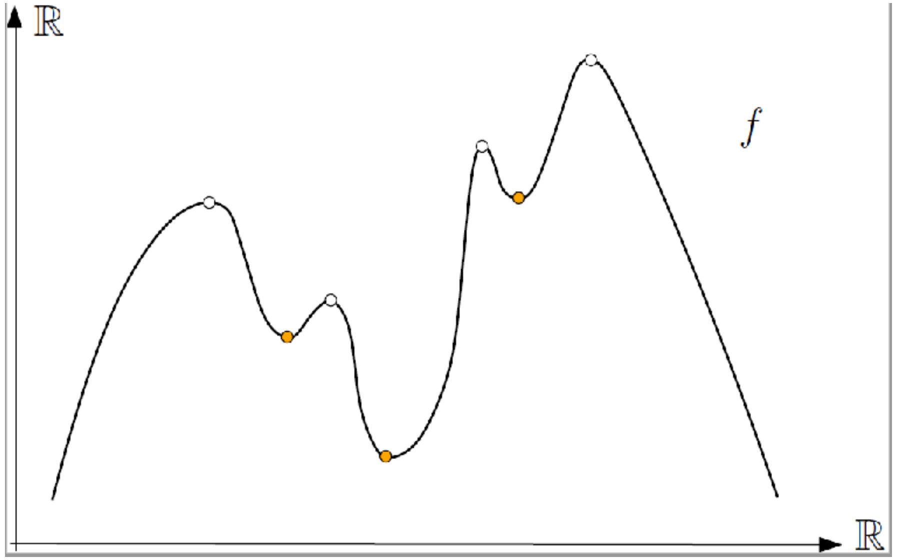
- Properties / attributes of data can often modeled as functions
- Characterize / summarize functions, as well as summarizing data themselves via this “function” perspective





Gradients and critical points

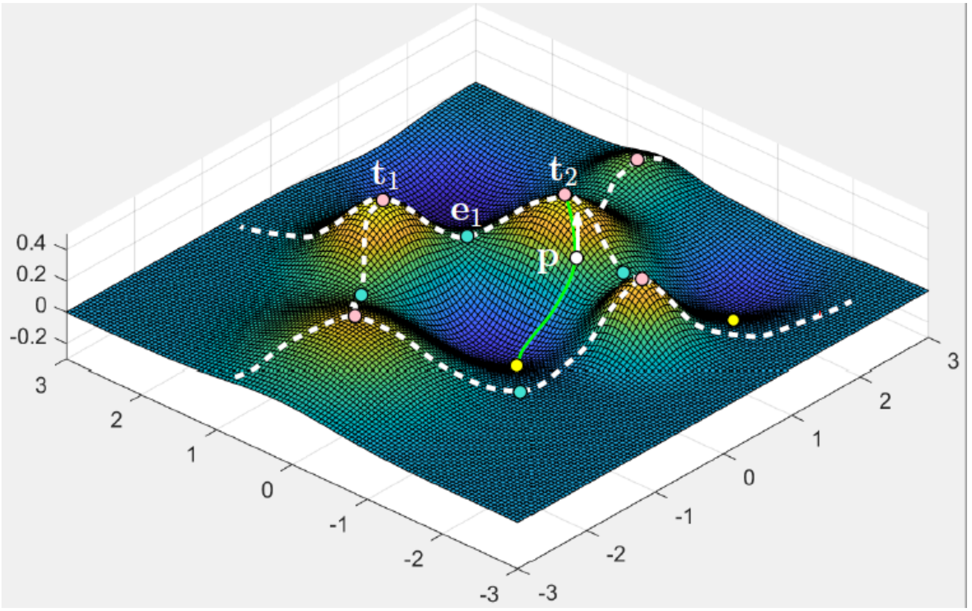
- 1D case: $f\colon \mathbb{R} \to \mathbb{R}$



- Derivative
  - $\nabla f(x) = \lim_{t \to 0} \dfrac{f(x+t) - f(x)}{t}$
  - measures rate of change
- Critical points:
  - A point $x \in \mathbb{R}$ is a *critical point* w.r.t. f if $\nabla f(x) = 0$
  - That is, critical points are where this derivative vanishes.
- A non-critical point is called a *regular point*.

Gradients, critical points

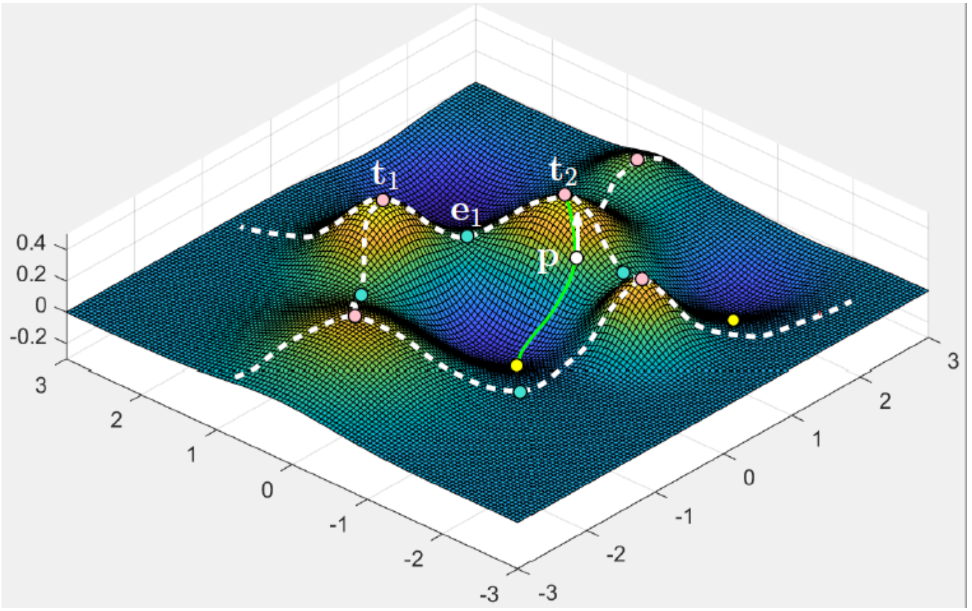
- dD case: $f\colon \mathbb{R}^d \to \mathbb{R}$



Gradients, critical points

- dD case: $f\colon \mathbb{R}^d \to \mathbb{R}$

- Directional derivative:
  - $D_v f(p) = \lim_{t \to 0} \frac{f(p + tv) - f(p)}{t}$
  - measures rate of change in direction v



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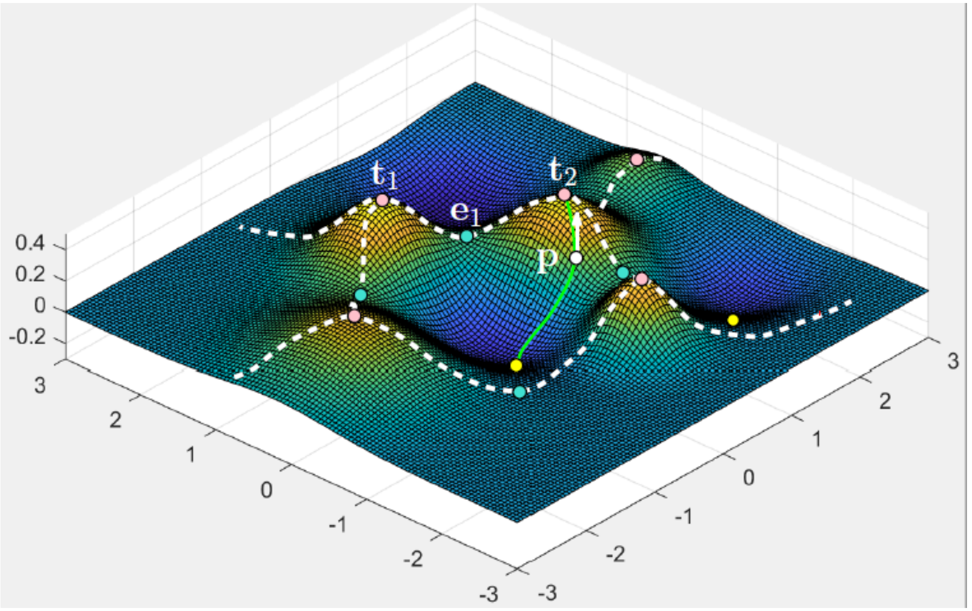

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  - $\nabla f(p) = \left[\frac{\partial f}{x_1}, \ldots, \frac{\partial f}{x_d} \right]^T$, where $x_1, .. x_d$ form an orthonormal coordinate system
    - It is in the direction with largest directional derivative (with steepest rate of increase)
    - The magnitude is that largest rate of increase.

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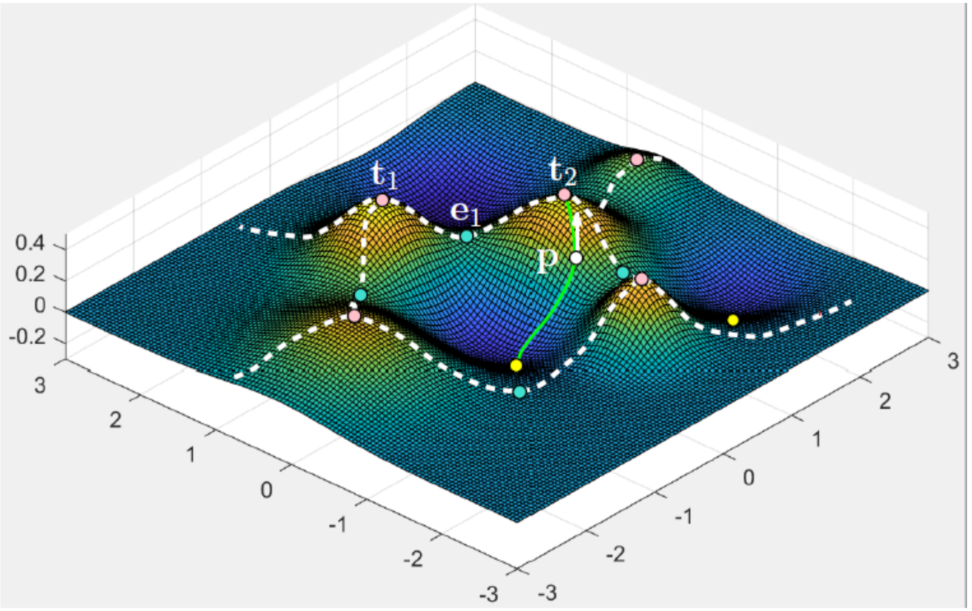

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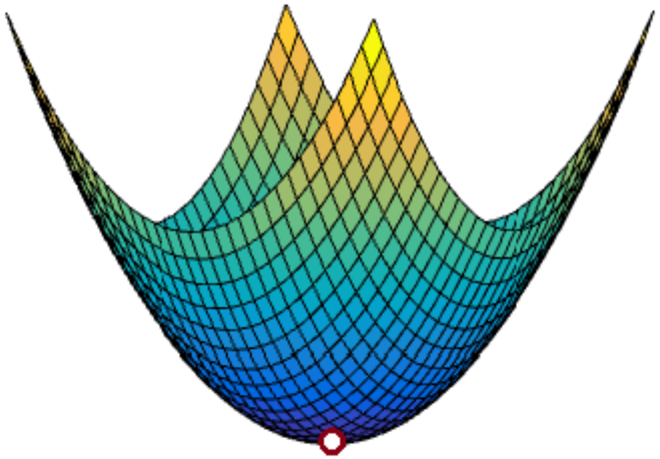
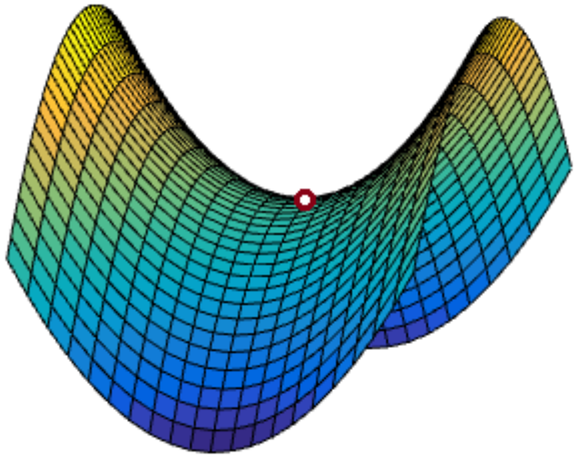
- Critical points:
  - A point p is *critical* if $\nabla f(p) = [0, \ldots, 0]^T$; that is, where gradient vanishes.

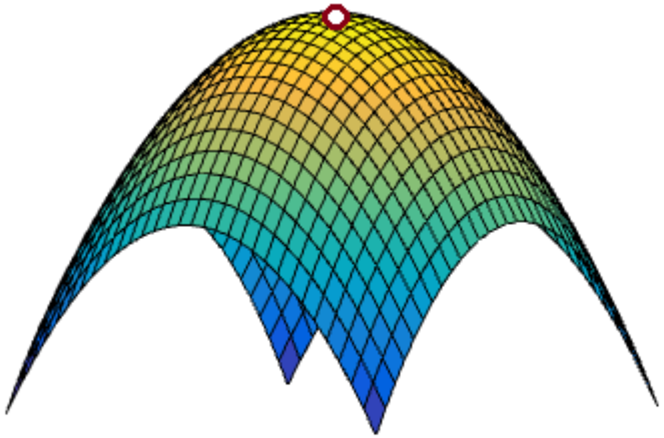
Examples for a 2D function



minimum

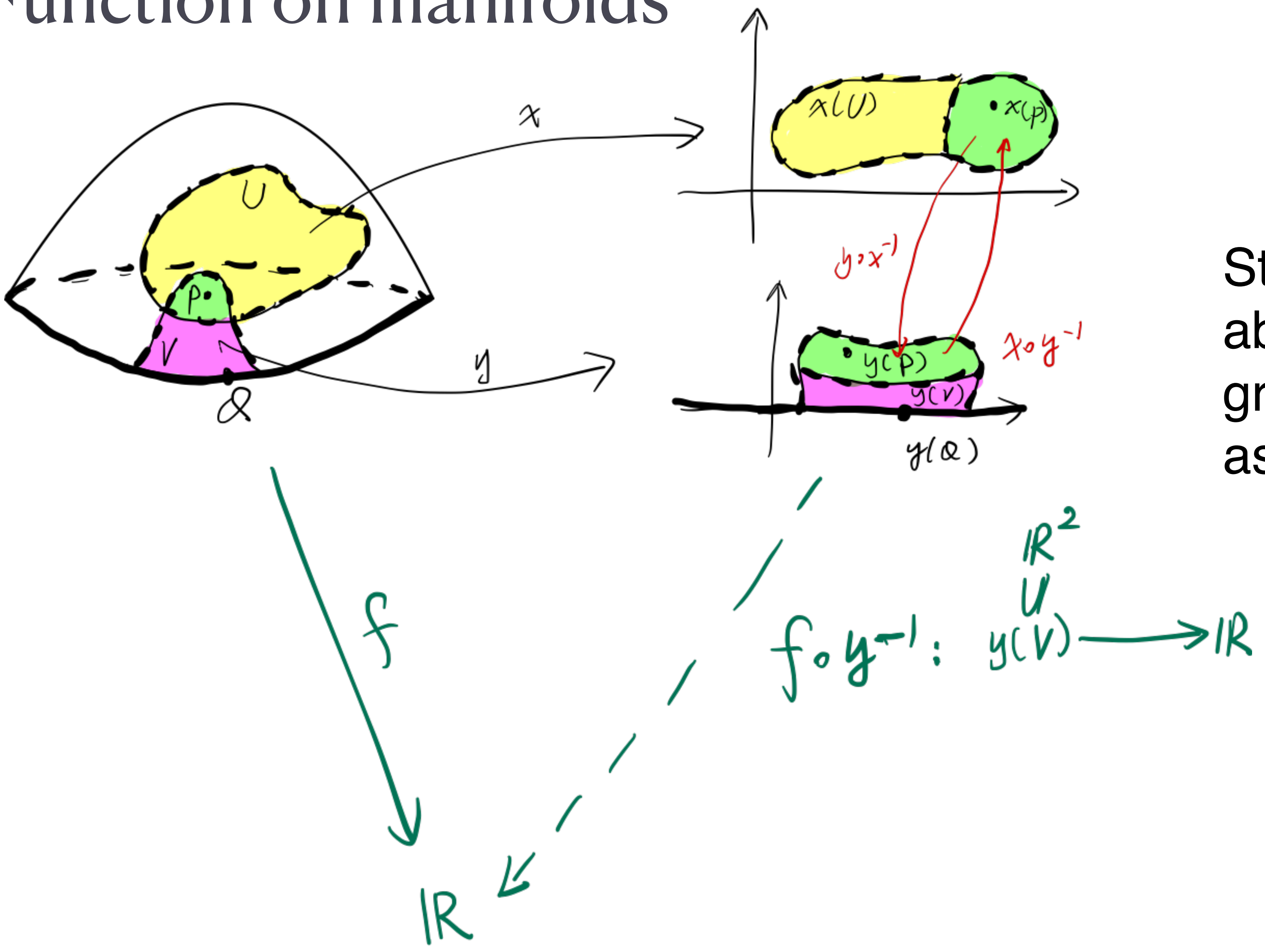


saddle



maximum

Function on manifolds



Still makes sense to talk about derivatives, gradients, critical points as they are local concepts

Gradients, critical points

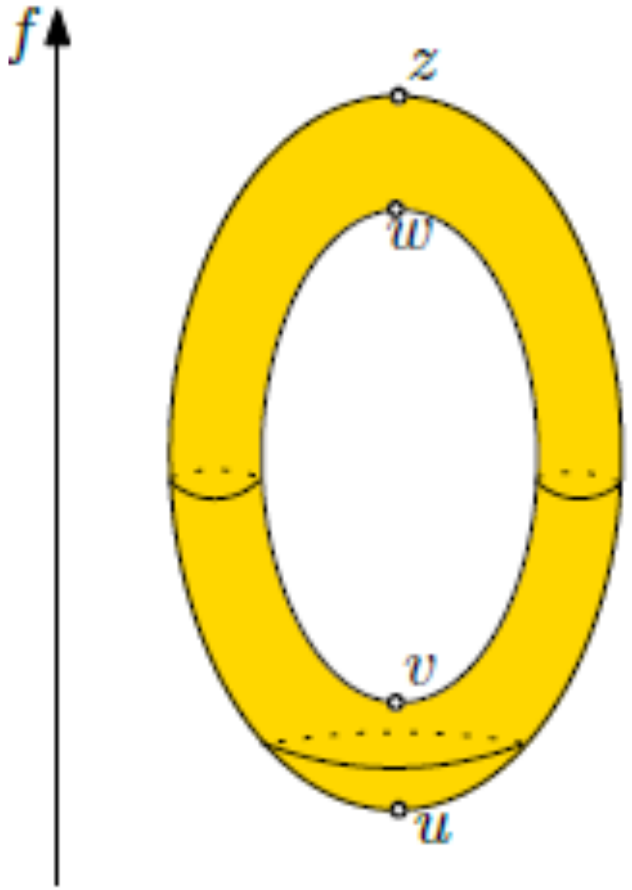
- d-manifold case: $f: M \to R$
- Same intuition, simply within a small neighborhood at each point

Definition 8 (Gradient vector field; Critical points)**.** Given a smooth function $f : M \to \mathbb{R}$ defined on a smooth m-dimensional Riemannian manifold M, the *gradient vector field* $\nabla f : M \to$ TM is defined as follows: for any $x \in M$, let $(x_1, x_2, \ldots, x_m)$ be a local coordinate system in a neighborhood of x with orthonormal unit vectors x_i, the gradient at x is

$$\nabla f(x) = [\frac{\partial f}{\partial x_1}(x), \ \frac{\partial f}{\partial x_2}(x), \ \cdots \ \frac{\partial f}{\partial x_m}(x)]^T.$$

A point $x \in M$ is *critical* if $\nabla f(x)$ vanishes, in which case $f(x)$ is called a *critical value* for f. Otherwise, x is *regular*.

Example



(Non-)degenerate critical points

Definition 9 (Hessian matrix; Non-degenerate critical points)**.** Given a smooth m-manifold M, the *Hessian matrix* of a twice differentiable function $f : M \to \mathbb{R}$ at x is the matrix of second-order partial derivatives,

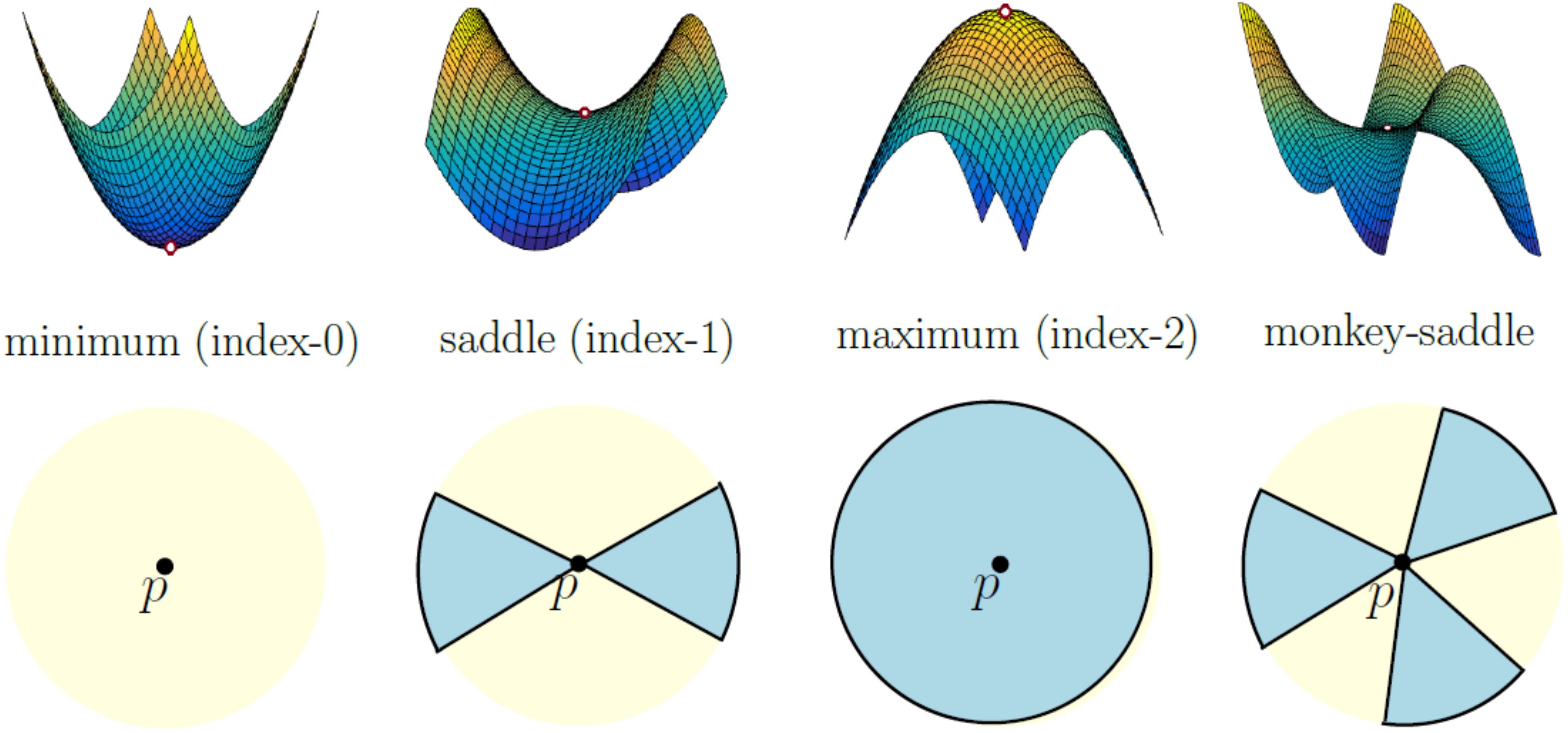
$$Hessian(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(x) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_m}(x) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_2}2(x) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_m}(x) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_m \partial x_1}(x) & \frac{\partial^2 f}{\partial x_m \partial x_2}2(x) & \cdots & \frac{\partial^2 f}{\partial x_m \partial x_m}(x) \end{bmatrix},$$

where $(x_1, x_2, \ldots, x_m)$ is a local coordinate system in a neighborhood of x.

A critical point x of f is *non-degenerate* if its Hessian matrix $Hessian(x)$ is non-singular (has non-zero determinant); otherwise, it is a *degenerate critical point*.

Number of negative eigenvalues is called the **index** of x

Examples


minimum (index-0)
saddle (index-1)
maximum (index-2)
monkey-saddle
p
p
p
p

Morse Function

Morse Function

- A smooth function is a Morse function if
  - (1) all critical points have distinct function values
  - (2) there is no degenerate critical point.
- Morse functions have well-behaved critical points!

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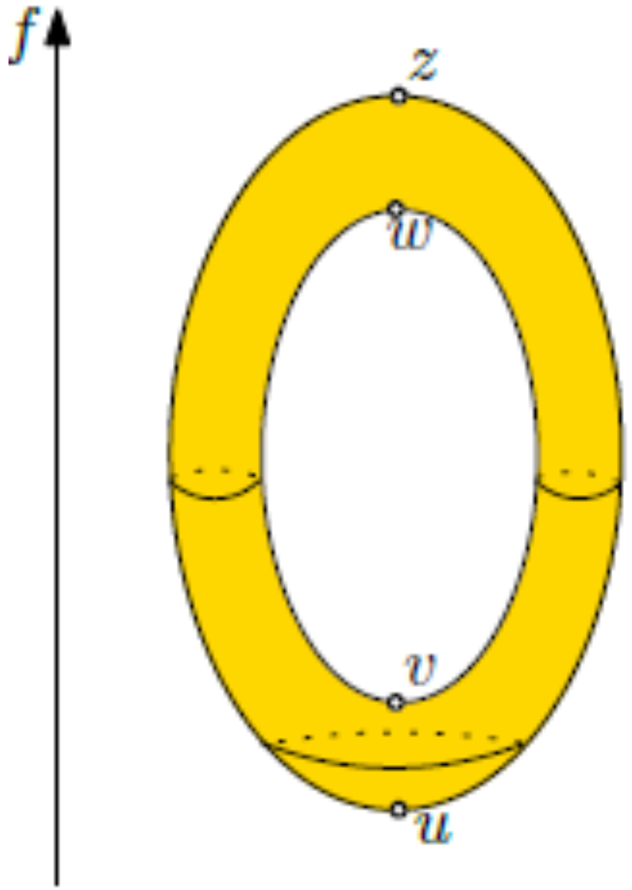
- Morse functions have well-behaved critical points!

Proposition 2 (Morse Lemma). *Given a smooth function $f : M \to \mathbb{R}$ defined on a smooth m-manifold M, let p be a non-degenerate critical point of f. Then there is a local coordinate system in a neighborhood $U(p)$ of p so that (i) the coordinate of p is $(0, 0, \ldots, 0)$, and (ii) locally for every point $x = (x_1, x_2 \ldots x_m)$ in neighborhood $U(p)$,*

$$f(x) = f(p) - x_1^2 - \ldots x_s^2 + x_{s+1}^2 \ldots x_m^2, \qquad \textit{for some} \quad s \in [0, m].$$

The number s of minus signs in the above quadratic representation of $f(x)$ is called the index of the critical point p.

Example

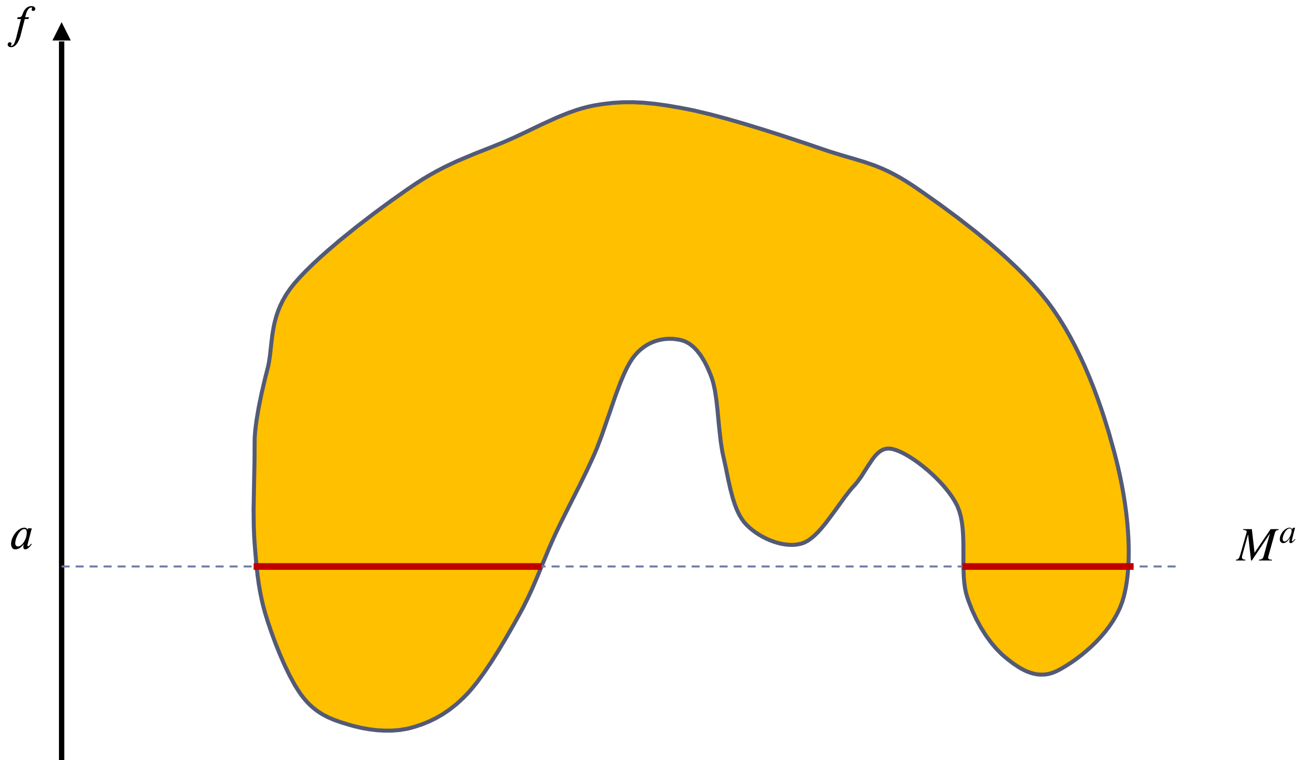


Why do we care about critical points?

- Intuitively, if we sweep the domain w.r.t. the function, this is where the topology of the swept portion changes.

Notations

- Function: $f: M \to R$
- Level set: $M^a = \{x \in M \mid f(x) = a\}$
- Sub-level set: $M^{\leq a} = \{x \in M \mid f(x) \leq a\}$
  - $M^{\leq a} \subseteq M^{\leq b}$ for any $a \leq b$



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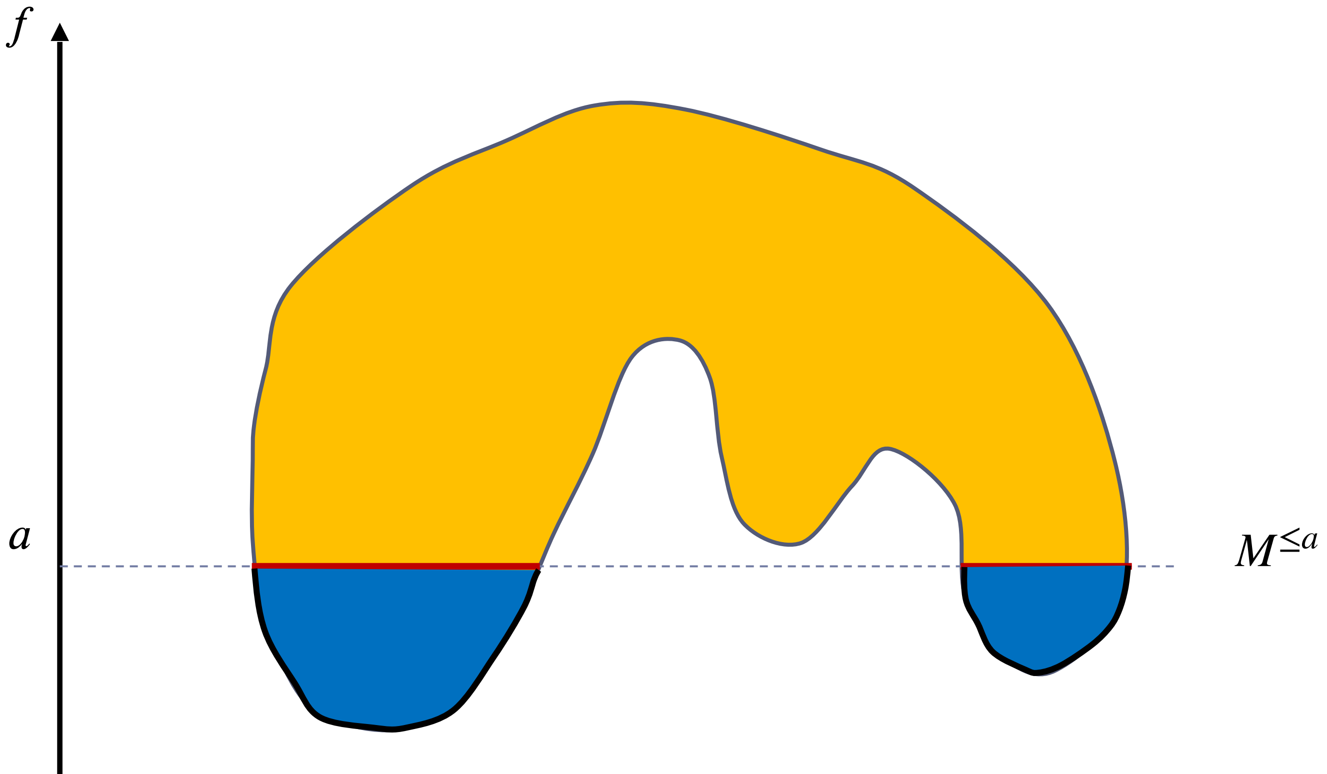

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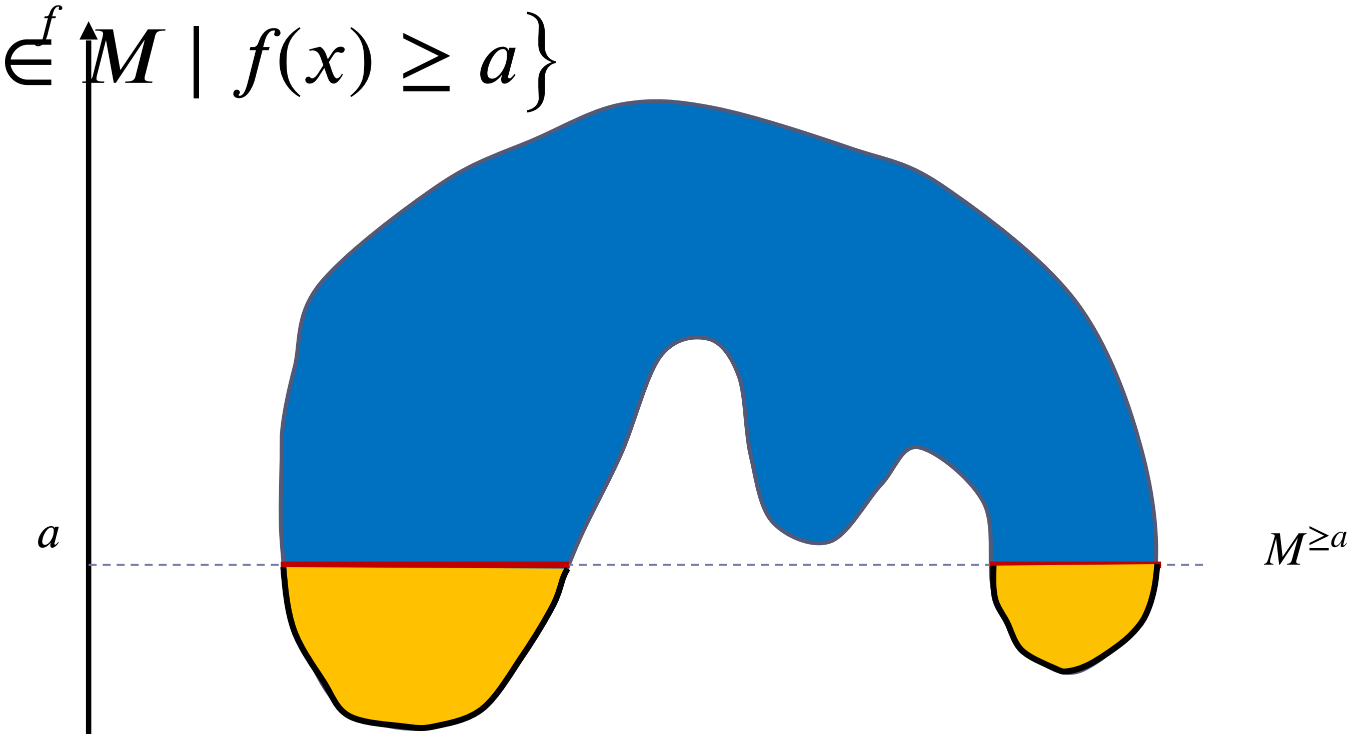

Critical points and topology

Theorem 3 (Homotopy type of sub-level sets)**.** *Let $f : M \to \mathbb{R}$ be a smooth function defined on a manifold M. Given $a < b$, suppose the interval-level set $M_{[a,b]} = f^{-1}([a, b])$ is compact and contains no critical points of f. Then $M_{\leq a}$ is diffeomorphic to $M_{\leq b}$.*

Furthermore, $M_{\leq a}$ is a deformation retract of $M_{\leq b}$, and the inclusion map $i : M_{\leq a} \hookrightarrow M_{\leq b}$ is a homotopy equivalence.

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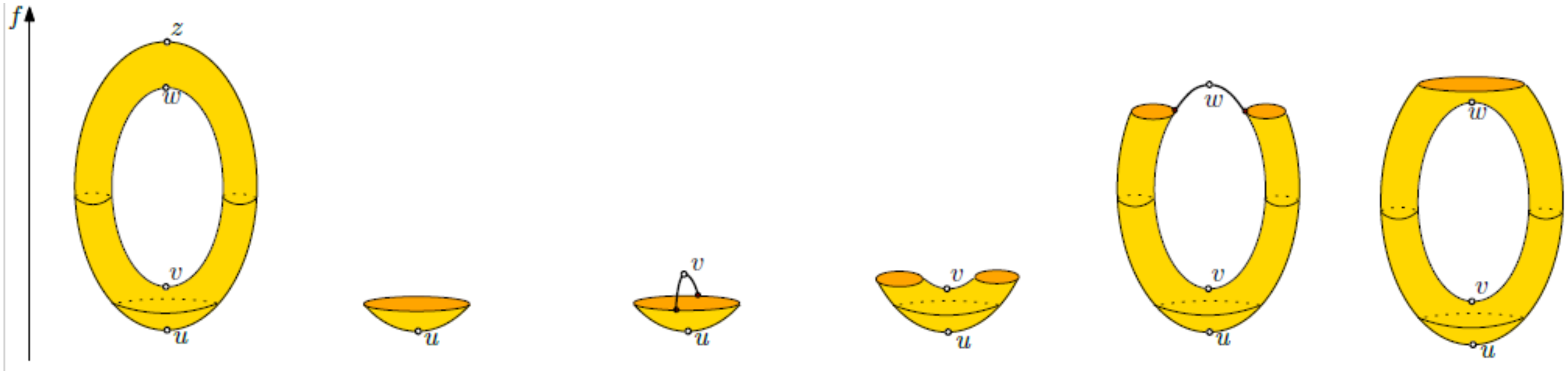

(a) (b) (c) (d) (e) (f)

Critical points and topology

Theorem 4. *Given a Morse function $f : M \to \mathbb{R}$ defined on a smooth manifold M, let p be an index-k critical point of f with $\alpha = f(p)$. Assume $f^{-1}([\alpha - \varepsilon, \alpha + \varepsilon])$ is compact for a sufficiently small $\varepsilon > 0$ such that there is no other critical points of f contained in this interval-level set other than p. Then the sublevel set $M_{\leq \alpha+\varepsilon}$ has the same homotopy type as $M_{\leq \alpha-\varepsilon}$ with a k-cell attached to its boundary $\mathrm{Bd}\, M_{\leq \alpha-\varepsilon}$.*

Animation

Critical points and topology

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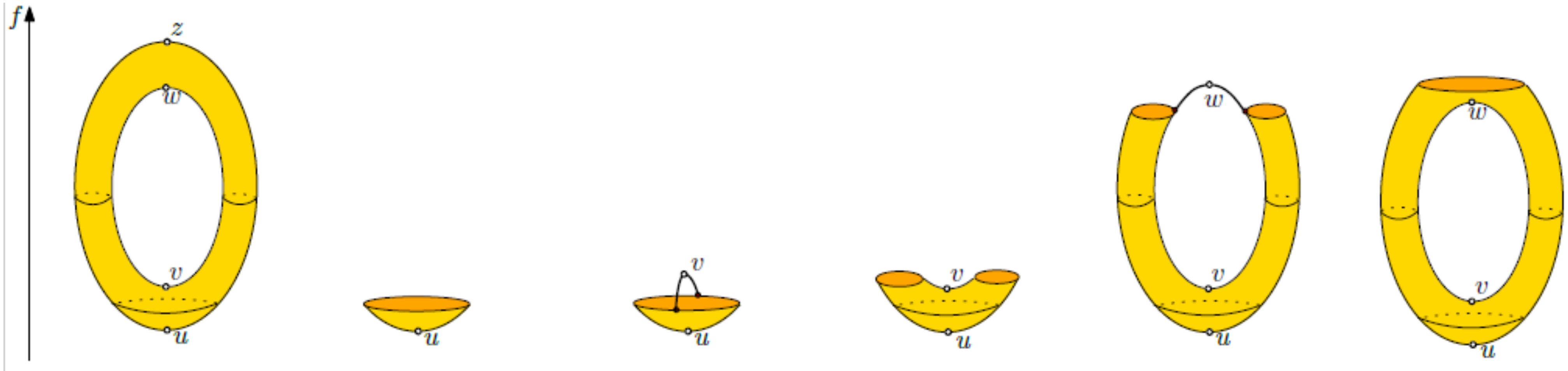
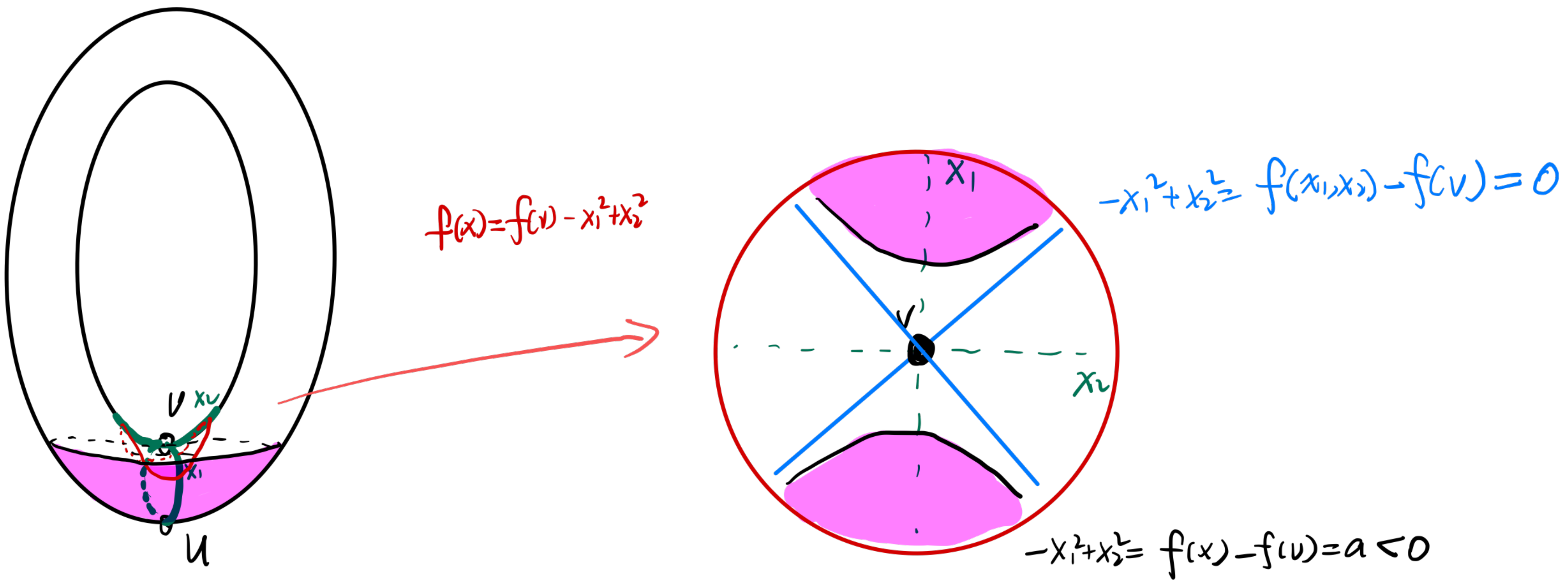


(a) (b) (c) (d) (e) (f)

Animation

Proof by picture



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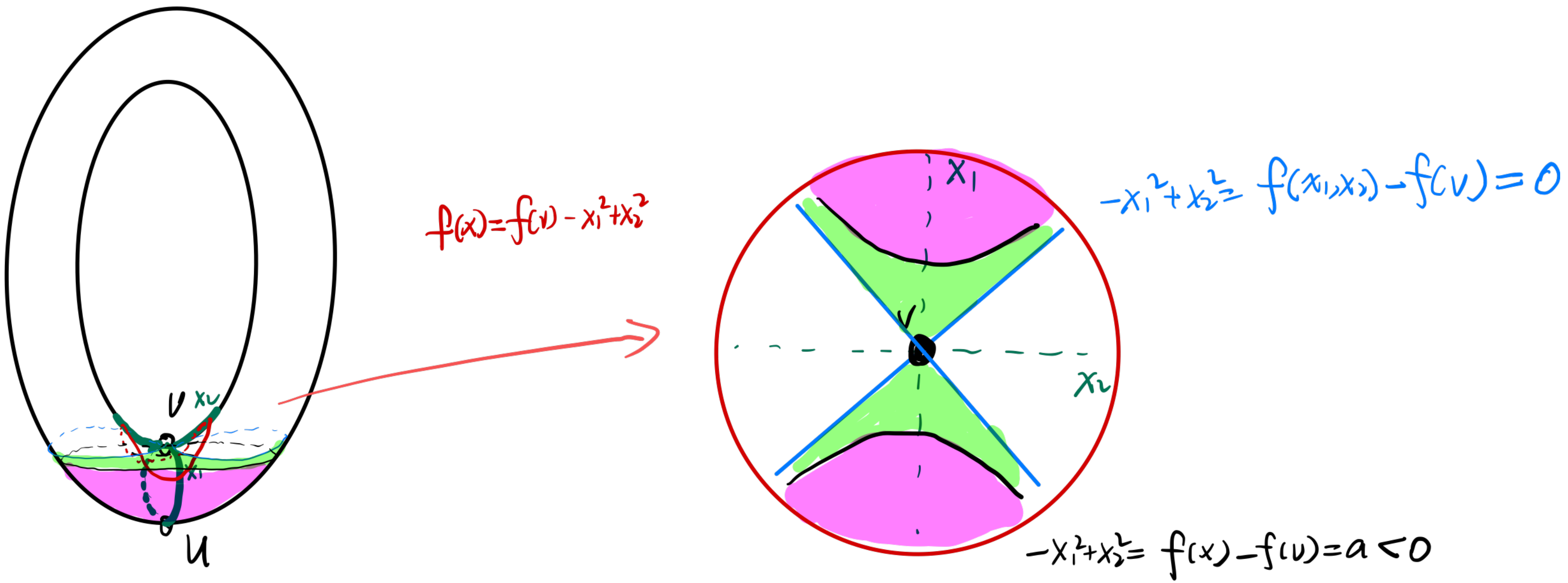

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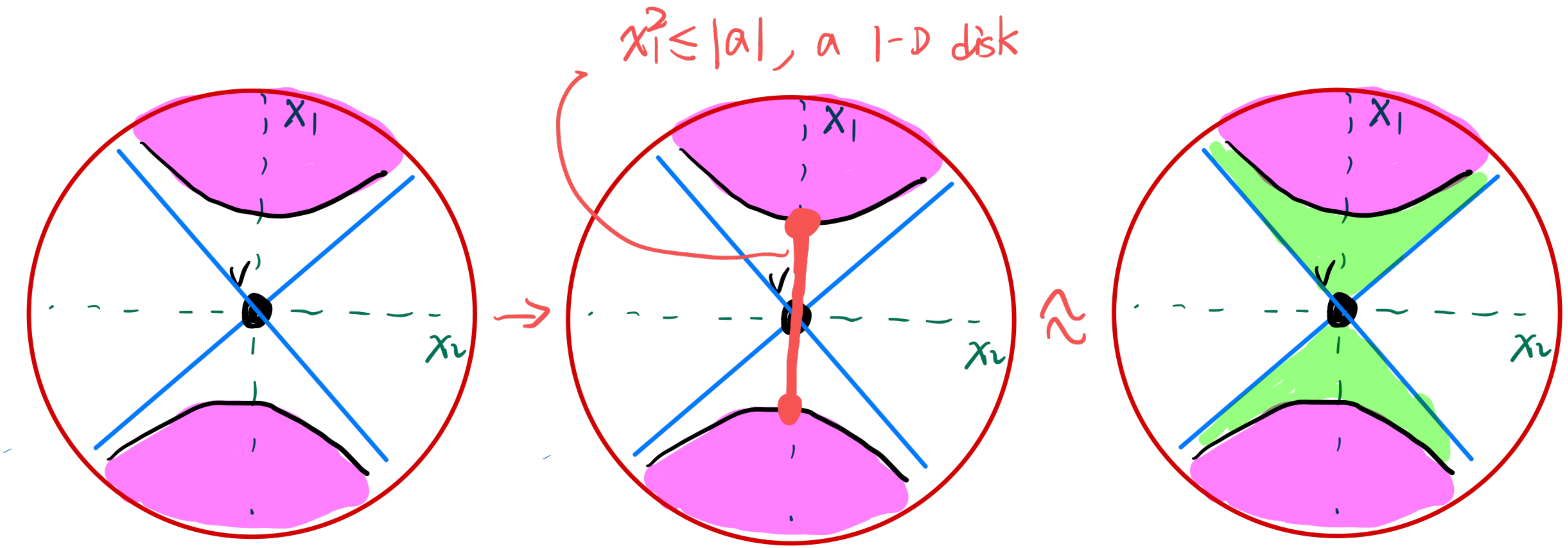

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