BIOMATH 208 Week 4

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Review

Curves and Surfaces

On a computer:

- list of points (vertices)
- list of connectivity elements (line segments, triangles)
  - Integers (2 for segment, 3 for traingle), which are indices for the array of vertices
  - orientation matters (we often want consistent tangent or normal vectors)

In a vector space:

- consider them as integral operators, compute path or flux integrals when acting on a smooth vector field.
- Therefore, these are covectors in the space dual to smooth vector fields
- We looked at the operator norm

$$|\delta|_{v^*} = \sup_{v \in V, |v|_v = 1} \gamma(v) = \|\gamma^\sharp\|_v$$

- We can model smooth functions instead of weird curves

We chose to use the reproducing kernel inner product for our space of smooth functions, and parameterize them as $v(x) = \sum_{i=1}^{N} p_i k(x - c_i)$. ($p_i$ is the direction, not normalized, and c_i is the center of the vector.), for any $N \in \mathbb{N}$.

- k as a gaussian with a fixed width

The reproducing kernel inner product is:

$$\langle ak(\cdot - a), bk(\cdot - y)\rangle_v = a \cdot bk(x - y)$$

- The $\cdot$ on the right hand side is a dot product in $\mathbb{R}^3$.
- This shows that non-smooth functions will have an infinite norm.

The Flat Map

While there are many objects included in the dual space, we will focus on the ones that result from the flat map.

The flat map is given by

$$\flat(aK(\cdot - x)) = a\delta_x$$

- K is a gaussian blob
- a is a vector
- x is a center

Definition (Linear evaluation functional)

δ_x acts linearly on a function, and returns its value at a point.

$$\delta_x(v) = v(x)$$

We define the action of $a\delta_x$ as

$$a\delta_x(v) = a \cdot v(x)$$

- The $\cdot$ is a dot product in $\mathbb{R}^3$.

The flat map for smooth vector fields

We can expand our definition using linearity

$$\flat\left(\sum_i a_i K(\cdot - x_i)\right) = \sum_i \flat(a_i K(\cdot - x_i)) = \sum_i a_i \delta_{x_i}$$

Proof

This flat map is the one defined by our inner product

$$\flat(aK(\cdot - x)) = a\delta_x$$

By the definition of inner product,

$$\begin{aligned}\langle ak(\cdot - x), bk(\cdot - y)\rangle_v &= a \cdot bk(x - y) \\ &= b(ak(\cdot - x))(bk(\cdot - y)) \\ &= a\delta_x(bk(\cdot - y))\end{aligned}$$

The Sharp Map

By definition, the sharp map is the inverse of the flat map:

$$\sharp(a\delta_x) = aK(\cdot - x)$$

It is extended to all ("nice") linear evaluation functionals by linearity.

Discrete Line Integrals

Approximate our curve γ with a sequence of points $x_1, \ldots, x_N$. The center of the ith edge is $c_i \frac{x_i + x_{i+1}}{2}$ for $i \in \{1, \ldots, N-1\}$. The tangent to the ith edge is $\tau_i = x_{i+1} - x_i$. Then:

$$\gamma(v) = \int v(\gamma(t)) \cdot \gamma'(t) \mathrm{d}t \simeq \sum_{i=1}^{N-1} v(c_i) \cdot \tau_i$$

- Centers: average of two consecutive points
- Tangent: difference between two consecutive points
- This is like a riemann sum.
- We can evaluate the right side of the equation (the summation) with evaluation functionals.

Integrals as evaluation functionals

We can rewrite this as:

$$\sum_{i=1}^{N-1} v(c_i) \cdot \tau_i = \left(\sum_{i=1}^{N-1} \tau_i \delta_{c_i} \right)(v)$$

The right side element $\left(\sum_{i=1}^{N-1} \tau_i \delta_{c_i}\right) \in V^*$, and is a discrete curve that can be written as a "nice" covector, a weighted sum of evaluation functions.

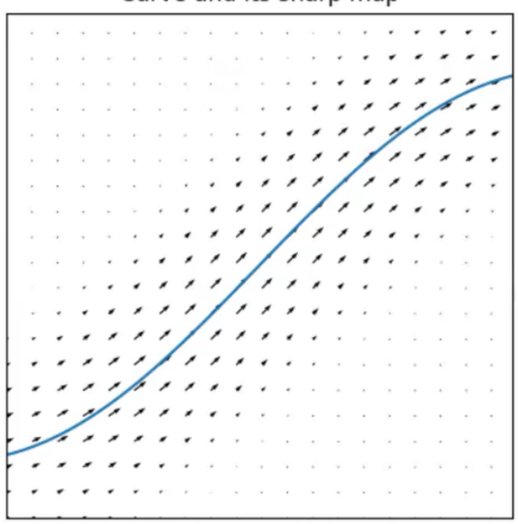
Sharp map for discrete curves

If γ is a discrete curve, then its sharp map is given by

$$\delta^\sharp(x) = \sum_{i=1}^{N} \tau_i K(x - c_i)$$

- We just replaced the δ_x with a K.
- In the below image, the vector field (black) is the sharp map applied to our curve.

Curve and its sharp map



Inner product for discrete curves

Let $\mu = \sum_{i=1}^{n^\mu - 1} \tau_i^\mu \delta_{c_i^\mu}$ and $\nu = \sum_{i=1}^{n^\nu - 1} \tau_i^\nu \delta_{c_i^\nu}$. The inner product is:

$$g_{V^*}(\mu, \nu) = \sum_{i=1}^{n^\mu - 1} \sum_{j=1}^{n^\nu - 1} K(c_i^\mu - c_j^\nu)(\tau_i^\mu \cdot \tau_j^\nu)$$

This equation works due to bilinearity, since

$$\langle \tau_1 \delta_{c_1}, \tau_2 \delta_{c_2} \rangle = \langle \tau_1 k(\cdot - c_1), \tau_2 k(\cdot - c_2) \rangle_v = \tau_1 \cdot \tau_2 k(c_1 - c_2)$$

The double sum we take in this formula represents the sum of all possible pairs of i and j. Think: nested for loops.

Distance between discrete curves

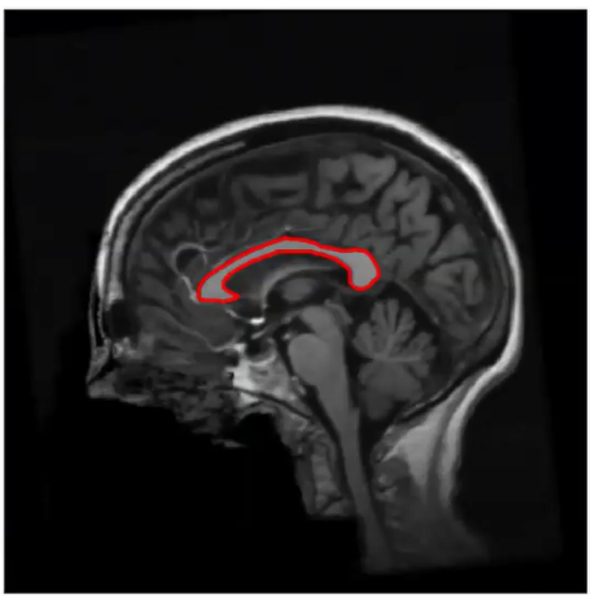
The distance between two curves is the norm of their difference.

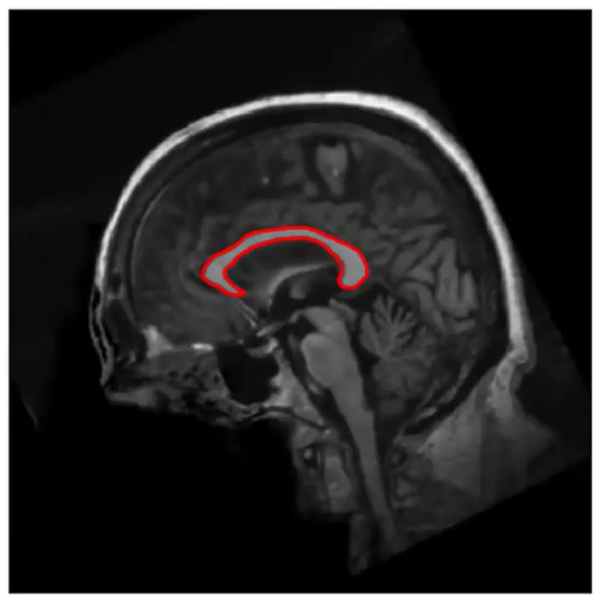
$$\begin{aligned}
&\|\mu - \nu\|^2_{V^*} \\
&= g_{V^*}(\mu,\mu) - 2g_{V^*}(\mu,\nu) + g_{V^*}(\nu,\nu) \\
&= \sum_{i,i'=1}^{n^\mu - 1} K(c_i^\nu - c_{i'}^\nu)(\tau_i^\nu \cdot \tau_{i'}^\nu) \\
&\quad - 2\sum_{i=1}^{n^\mu - 1}\sum_{j=1}^{n^\nu - 1} K(c_i^\mu - c_j^\nu)(\tau_i^\mu \cdot \tau_j^\nu) \\
&\quad + \sum_{j,j'=1}^{n^\nu - 1} K(c_j^\nu - c_{j'}^\nu)(\tau_j^\nu \cdot \tau_{j'}^\nu)
\end{aligned}$$

We are essentially summing

- All the pairs in the first curve, $g_{V^*}(\mu,\mu)$,
- all the pairs between the two curves, $2g_{V^*}(\mu,\nu)$,
- and all the pairs in the second curve, $g_{V^*}(\nu,\nu)$

The Corpus Callosum





- One of the most visible and well-studied parts for the brain is the Corpus Callosum, because it contains such a large amount of white matter
- In the past, a common treatment for epilepsy was to sever the Corpus Callosum, as it prevents positive feedback loops between the two sides.
- Its shape changes depending on different diseases, phenotypes, etc.

Review - Curve Fitting and Interpolation

Consider a curve fitting problem: You have a lot of data points. The goal is to find a "nice" $f(x)$ that passes through my data.

What does "nice" mean? It is a curve with no cusps or discontinuities.

To do this, we first find the minimizer of f.

$$\text{argmin}_{f \in V} \langle f, f \rangle_v \text{ such that } f(x_i) = y_i \qquad \forall i \in \{1, \ldots, N\}$$

This is a costumed plurization, use Lagrange multipliers p_i.

$$\begin{aligned} L &= \sum_{i=1}^{N} p_i \cdot (y_i - f_i) + \langle f, f \rangle_v \\ &= \sum_{i=1}^{N} p_i f(x_i) + \frac{1}{2} \langle f, f \rangle_v + \sum_{i=1}^{N} p_i y_i \end{aligned}$$

for a fixed p, find the best f. (Notice the last term in the above equation is not dependent on f.)

$$\begin{aligned} &= \sum_{i=1}^{N} P_i \delta_{x_i}(f) + \langle f, f \rangle_v + \sum_{i=1}^{N} p_i y_i \\ &= \langle \sum_{i=1}^{N} p_i \cdot K(\cdot - x_i), f \rangle_v + \langle f, f \rangle_v + \cdots \\ &= \langle g, f \rangle_v + \langle f, f \rangle_v + \cdots \end{aligned}$$

We can solve this by completing the square. The result would look something like

$$\langle f - g, f - g \rangle_v + \cdots$$

The constants of this equation are independent of f. This equation is minimized when $f = g$.

Therefore, the optimal f is $f(x) = \sum_{i=1}^{N} p_i K(x - x_i)$.

- We now need to solve for p.
- In these types of problems, p is a lagrange multiplier, so we would have to refer to the constraints.

$y_j = f(x_j) = \sum_{i=1}^{N} p_i K(x_j - x_i)$

- p_i is a N by 1 array
- $k(x_j - x_i)$ is an N by N array.
- Therefore, the right side can be thought of as matrix multiplication.

solve for p by solving linear equations!

Smooth Manifolds

Motivation: Many useful data types in medical imaging are not elements of a vector space. (Not closed under $+$ and $\cdot$.)

- Rotation matrices

- Diffusion tensors
- Probabilities

We can still analyze them quantitatively by modeling them as elements of a manifold.

We will discuss two main types of data

1. Pixels that are manifold valued objects
2. Manifold valued objects that act on imaging data

Intuition for Smooth Manifolds

A manifold is a set (possibly curved), such that if you zoom in close it looks like a (flat) vector space (i.e., $\mathbb{R}^d$ for some d).

- A classic example is a sphere like the earth. When we walk around in a small area it looks flat.

Example - Not Manifolds

1. A line segment:
   - Imagine you are standing at the end of a line segment. You see a cliff! The segment ends, but $\mathbb{R}$ doesn't.
2. An "x":
   - Consider the intersection between two lines. If you zoom in on the intersection, it always looks the same! It does not smooth out.

Definition of a Smooth Manifold

A smooth manifold is a triple

1. A set $\mathcal{M}$
2. A topology $\mathcal{O}$
3. A collection of smoothly compatible charts called an atlas $\mathcal{A}$, where every point is in at least one chart.

Topologies

- We will not cover topologies in detail in lecture. Please see the notes if you are interested.

Working definition of topologies: We can think of a topology as a collection of open sets (including $\mathcal{M}$ and $\emptyset$), that allow us to define continuous functions:

- A function f is continuous if the inverse image of any open set is also open set.

Charts

Charts will make precise what "looks like $\mathbb{R}^d$ means. Definition: A chart is a pair (U, x) in $\mathcal{A}$, where U is an open subset of $\mathcal{M}$ and $x : \mathcal{M} \to \mathbb{R}^d$ is a continuous and invertible map, with continuous inverse (a homeomorphism), called the coordinate map, for some $d \in \mathbb{N}$. Definitiion: d is called the dimension of the manifold.

Components

Definition: We call x^i the i-th component map. It can be thought of as first applying x, then identifying the i-th component in a basis $x^i = \epsilon^i \circ x$. Note components have an index up!

- We will always choose a standard basis for ϵ^i.
- x will input a point on the manifold and output a list of d numbers
  - Each item on the list is a component.
- Note that a set here refers to a set of functions (which vary with p, the point picked), rather than a basis which is a set of vectors.

Example: The Open Interval

Consider the interval $(0, 1) \in \mathbb{R}$. We can choose x as the "natural" chart. If $p \in \mathcal{M}$m then $x(p) = p$, and the domain is all of $\mathcal{M}$

- We are essentially choosing $x(p)$ as a point on a number line from 0 to 1. We can represent $x(p)$ by the number p.

Or we could use the logit (log of odds) chart, $y(p) = \log\left(\frac{p}{1-p}\right)$. The domain is again all of $\mathcal{M}$, and the image is all of $\mathbb{R}$.

- In these lectures, log refers to natural log.

Note the inverse:

- If we represent data this way, we don't have to worry about constraints.

$$y'(q) = \frac{1}{1 + e^{-q}}$$

- This is a (sigmoid) logistic function, derived from the $y(p)$ equation above, setting $y(p) = q$, and solving for p.
- Any function can be used, this is just an example, as long as the function has a domain from 0 to 1, and is continuous.

Example: The Plane

Consider the ordered tuples in $\mathbb{R}^2$. We could use the "natural" chart with $x(p) = 0$. Here, $x^0(p) = p^0$, and $x^1(p) = p^1$. The domain is all of $\mathcal{M}$.

Or, we could consider rotated and translated charts.

$$\begin{aligned} y^0 &= \cos(\theta)p^0 + \sin(\theta)p^1 + h \\ y^1 &= -\sin(\theta)p^0 + \cos(\theta)p^1 + k \end{aligned}$$

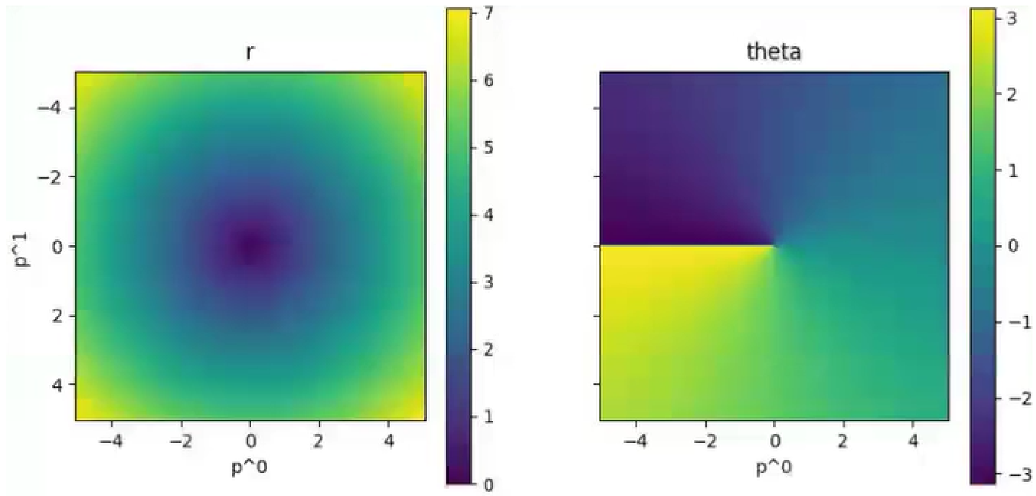
for $\theta \in [0, 2\pi]$ and $h, k \in \mathbb{R}$.

- (h, k) is a shift, θ is a rotation.
- Given one chart, we could immediately construct an infinite amount of new charts!
- Our atlas and charts will never be unique.

Or, we could consider the "polar" chart, with

$$z(p) = \left(\sqrt{(p^0)^2 + (p^1)^2}, \operatorname{sign}(p^1) \arccos \left(\frac{p^0}{\sqrt{(p^0)^2 + (p^1)^2}} \right) \right)$$

- This coordinate, $z(p)$ is in the format, (radius, angle).



Here, the domain is $U = \mathbb{R}^2$, minus the "nonpositve x-axis". Since it doesn't cover $\mathcal{M}$, this can't be the only chart in our atlas.

- Notice that the theta graph is noncontinuous. Also at the origin, it is not invertible.

Example: The Circle

Consider a circle with radius 1, centered at the origin in the Cartesian plane:

$$S = \{p \in \mathbb{R}^2 \ : \ (p^0)^2 + (p^1)^2 = 1\}$$

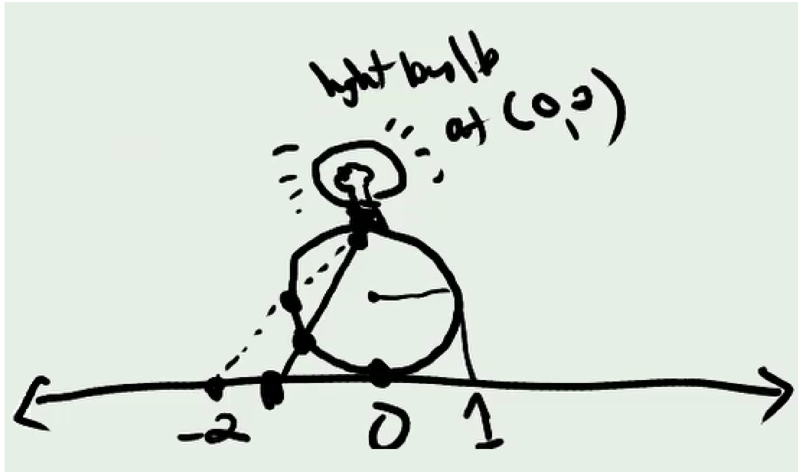
We will cover the circle with two "polar" charts.

First, $U = S \backslash (-1, 0)$, $x(p) = \operatorname{sign}(p^1) \arccos(p^0)$. This is the signed angle counterclockwise from positive x-axis.
Second, $V = S \backslash (0, -1)$, $y(p) = \operatorname{sign}(p^0) \arccos(o^1)$. Signed angle clockwise from positive y-axis.

- The backslash ($\backslash$) represents subtraction of sets.
  - e.g., U covers every point on the circle except (-1, 0).
- With these two definitions, $U \cup V = \mathcal{M}$. This makes a nice atlas for the circle using continuous and invertible functions.

For another insightful pair of charts, consider the circle sitting on the real line, with a lightbulb on top. We assign a coordinate where our point casts a shadow. For points in $U = S \backslash (0, 1)$, we have

$$z(p) = \frac{2p^0}{1 - p^1}$$



- Here, the bottom half of the circle would cause a shadow between $-2 < x < 2$, and the points on the top half of the circle going to infinity on both sides
- The only point not responsible for a shadow is (0, 2)

This gives insight as to the meaning of $\pm\infty$! It's just the one point missing from the top of the circle.

- Importantly, this mapping maps all of $\mathbb{R}$ to a circle! (With one point gone).

Question: Can the circle be covered with one chart?

Answer: NO!

This is pretty easy to prove. Suppose that there is a function x that maps a circle to $\mathbb{R}$, which is continuous and invertible on the whole circle.

- Consider if you remove one point from the circle.
- The circle is still a connected set, with one point removed.
- However, $\mathbb{R}$ must have a discontinuity if the point was removed.
- Since continuity is always preserved by all continuous functions, the function must not be continuous. This is a contradiction, and therefore, the mapping cannot exist.

Example: The Hemisphere

Consider the surface of a human skull as a hemisphere,

$$\mathcal{M} = \{p \in \mathbb{R}^3 \, : \, (p^0)^2 + (p^1)^2 + (p^2)^2 = 1, p^2 > 0\}$$

Example: Parallel Projections

Imagine a camera high above the patient's head, recording their skull with a video camera. Points on the head will map to the screen using their "xy coordinate". This chart can be written as (U, x), where $U = \mathcal{M}$, and $x(p) = (p^0, p^1)$.

- The head will look like a circle.
- We don't consider the boundary of the head as part of our set, because it will not be a function with respect to the z-axis.

- Essentially, the sides of the head are perpendicular to our camera's view, which violates the vertical line test.

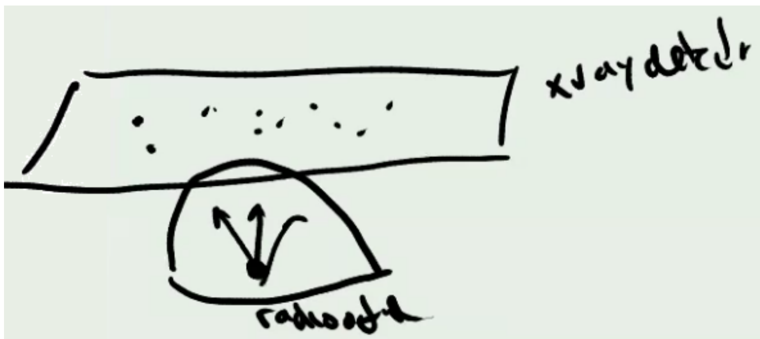
In this case, the inverse of $x(p)$ can be written as:

$$x^{-1}(q) = (q^0, q^1, \sqrt{1 - (q^0)^2 - (q^1)^2})$$

The z-coordinate represents the height of the pixel.

Example: Xray Projection

Imagine a radiotracer in the center of their head. A detector (the plane $p^2 = 1$) lies above their head and forms an image of their skull. This corresponds to the chart (V, y), where $V = \mathcal{M}$ and $y = (p^0/p^2, p^1/p^2)$



Note this maps he hemisphere to all of $\mathbb{R}^2$, in a similar way the lightbulb on a circle worked.

Example: Latitude and Longitude

Since this is a hemisphere (like part of the earth), it might be natural to work with latitude and longitude. This corresponds to the chart (W, z), where $W = \mathcal{M}\setminus$ "nonpositve x axis", and

$$z = \left(\frac{\pi}{2} - \arccos(p^2), \operatorname{sign}(p^1) \arccos(\frac{p^0}{\sqrt{(p^0)^2 + (p^1)^2}}) \right)$$

This cannot be our only chart.

Summary

We build three very different charts to describe the same (hemisphere) object. First we thought of the hemisphere as a graph of a function of two variables. Then, a map onto all of $\mathbb{R}^2$. Then, a map onto a finite subset of $\mathbb{R}^2$. (angles)

Example: The Sphere

The sphere also cannot be covered with one chart. One classic approach is to cover it with 6 parallel projection hemisphere charts.

- $+x, -x$
- $+y, -y$
- $+z, -z$

Another is latitude and longitude (as above), but we'll have to choose two neighborhoods.

Another choice is to place a light on the north pole, and cast the shadow of a point onto the plane:

$$x(p) = (2p^0/(1-p^2), 2p^1/(1-p^2))$$

with U the sphere minus the north pole.

A fun choice is to use the arcsine function sine $p^i \in (-1, 1)$, $(\mathcal{M}, y)$ where $y = (\arcsin(p^0), \arcsin(p^1))$

- You end up with the same problem with the lightbulb on the circle.

Atlases

An atlas is a collection of charts (coordinate neighborhood and homeomorphism to $\mathbb{R}^2$), such that every point on the manifold is in at least one chart.

Chart Transition Maps

This is essentially a change of basis. For any two chart (U, x), (V, y) with $U \cap V \neq \emptyset$, the mappings $x \circ y^{-1}$ and $y \circ x^{-1}$ are called chart transition maps. Note these are maps from $\mathbb{R}^d \to \mathbb{R}^d$. There is no $\mathcal{M}$ involved, and these can be studied with regular calculus.

Compatible Atlases

For a property $\mathcal{P}$, two charts x and y are called $\mathcal{P}$-compatible if $x \circ y^{-1}$ and $y \circ x^{-1}$ have the property $\mathcal{P}$. If every chart transition map has property $\mathcal{P}$, this is called a $\mathcal{P}$-compatible atlas.

Smooth manifolds

A smooth manifold is one where every chart transition map is a smooth map. That is, its derivative is a smooth function from $\mathbb{R}^d \to \mathbb{R}^d$.

- We want continuous derivatives so we can do gradient based optimization.

Example: The Interval

Example: Smoothly Compatible Charts

Using two charts: $(, x)$ and (V, y), with $x(p) = p$ and $y(p) = \log(p/(1-p))$, we have:

- $x \circ y^{-1}(u) = \frac{1}{1+e^{-u}}$
- $y \circ x^{-1}(u) = \log \frac{u}{1-u}$

These are both smooth maps from $\mathbb{R} \to \mathbb{R}$.

Example: Incompatible Atlas

Consider a second chart (W, z), with $z(p) = p^3$ in addition to the first chart, $x(p) = p$. Then,

- $x \circ z^{-1}(u) = u^{1/3}$
- $z \circ x^{-1}(u) = u^3$

These are not both differentiable everywhere.

Example: The Plane

Example: Smoothly Compatible Charts

Consider the identity chart (U, x) for $U = \mathcal{M}$ and $x(p) = 0$, and the polar chart (V, y) for $V = \mathcal{M}\backslash$ "nonpositive x axis" and $y(p) = \left(\sqrt{(p^0)^2 + (p^1)^2}, \operatorname{sign}(p^1) \arccos(p^0/\sqrt{(p^0)^2 + (p^1)^2})\right)$. Then,

- $y \circ x^{-1} = y(p)$ (as defined above)
- $x \circ y^{-1} = (r\cos(\theta), r\sin(\theta))$, or the inverse of $y(p)$.

These are differentiable everywhere except for the slit we cut out.

Example: The Hemisphere

Compatible Charts on the Hemisphere

Consider (U, x) parallel projection, and (V, y) arcsine angles.

First, find the inverse of parallel projection

$$x^{-1}(u) = (u^0, u^1, \sqrt{1 - (u^0)^2 - (u^1)^2})$$

Then the inverse of arcsine angles

$$y^{-1}(u) = (\sin u^0, \sin u^1, \text{height})$$

Example: Chart Transition Maps 1:

Consider the map $y \circ x^{-1}$:

$$(x^1, x^0) \to (\arcsin(x^1), \arcsin(x^2))$$

The derivatives are a 2x2 (diagonal) matrix:

$$\begin{pmatrix} \frac{1}{\sqrt{1-(x^1)^2}} & 0 \\ 0 & \frac{1}{\sqrt{1-(x^2)^2}} \end{pmatrix}$$

Similarly, this does not include the boundary.

Example: Chart Transition Maps 2:

Consider the map $x \circ y^{-1}$:

- x is the parallel projection, and y is the sines.

$$(y^1, y^2) \mapsto (\sin(y^1), \sin(y^2))$$

The derivatives are again a 2x2 (diagonal) matrix.

$$\begin{pmatrix} -\cos(y^1) & 0 \\ 0 & -\cos(y^0) \end{pmatrix}$$

This function exists everywhere. This matrix is continuous and invertible, there it is a smoothly compatible atlas.

- A hemisphere with this choice of atlas is a smooth manifold.

Extrinsic Coordinates

Often we will consider manifolds that are subsets of a larger space, such as surfaces in 3D, or matrix groups in $\mathbb{R}^{3\times 3}$.

It is natural to associate each $p \in \mathcal{M}$ as a point, an "extrinsic coordinate" (e.g., a point in 3D), as well as a chart (e.g., a coordinate in 2D).

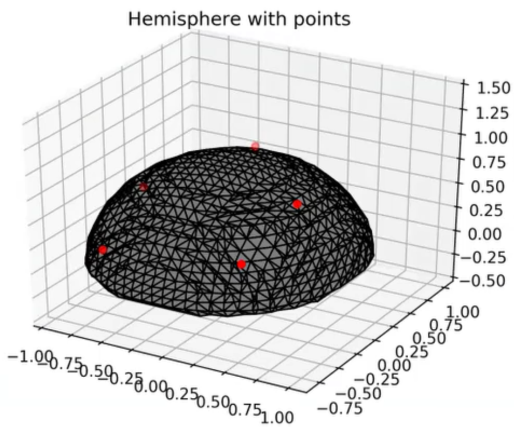
A danger is that the result of computations may not lie in the manifold.

Averages

Example: Points on a hemisphere

Find the average of 5 points on a hemisphere.

```
[ 0.512 -0.725  0.461]
[-0.221  0.63   0.744]
[-0.538 -0.776  0.329]
[-0.907  0.27   0.325]
[ 0.598 -0.172  0.783]
```



The easiest way is the way we were taught in middle school - add them up and divide by n. This is the **average in extrinsic coordinates**.

- Summing all the coordinates and dividing by 5 gives `[-0.111, -0.155, 0.528]`.
- Note the distance of this point from the origin is 0.562, so it is not on the hemisphere.
- Therefore, this calculation is inappropriate!

Example: Parallel Projection

Project all the points onto the x, y-plane. In this case, we just drop the z-coordinate.

- Finding the average this way (dropping z, summing points and dividing by 5), gives `[-0.111, -0.155, 0.982]`. The first two cooridnates are the same as before, except the z coordinate is picked so it is on the hemisphere.
- This is a better answer.

Example: Angular Coordinates

For this one, we use the angle from the north pole and the angle from the x-axis. This gives the following (five, 2D) coordinates:

```
[[ 0.479,  0.839,  0.335,  0.331,  0.9  ]
 [-0.956,  1.908, -2.177,  2.853, -0.281]]
```

and the following average: `[0.577, 0.269]`, which, converting back to cartesian coordinates, corresponds to the 3D point `[0.808, 0.223, 0.545]`.

- This is another different answer.
- The first answer (straight average) is wrong. The other two may be useful, depending on the case.