Shape Matching: A Metric Geometry Approach

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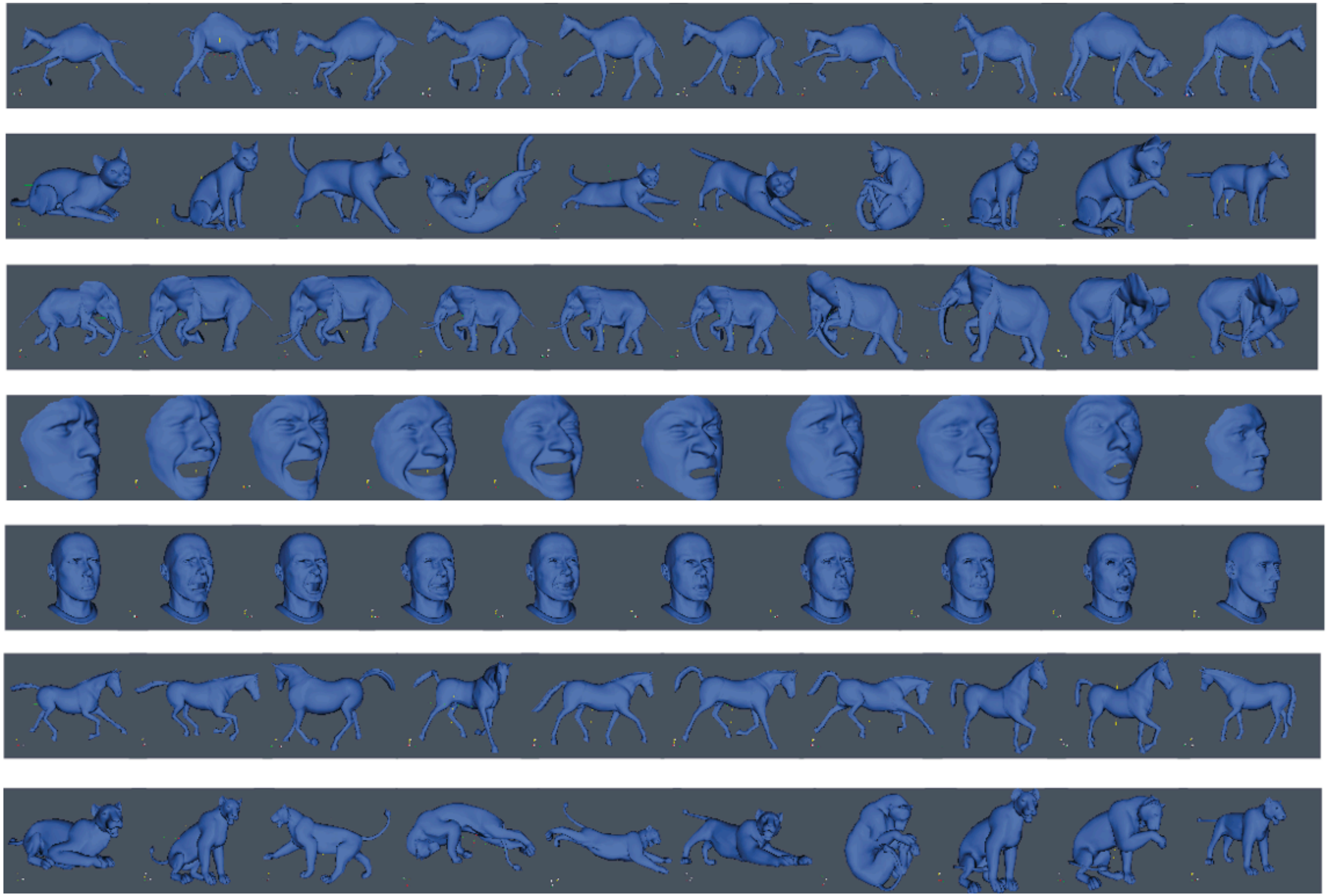
CS 468, Stanford University, Fall 2008.

General stuff:

- class attendance is mandatory
- will post possible projects soon
- a couple of days prior to each class i will update the webpage and post materials you should read on your own, before the class.
- you should read the papers so as to gain basic understanding of the idea proposed by the authors
- in my slides i will use the following tags for the materials listed under the"resources" section of the class webpage:
  - [**BBI**] will refer to the AMS book by Burago, Burago and Ivanov.
  - [**Villani**] AMS book by Cedric Villani.
  - [**M07**] my PBG07 paper.

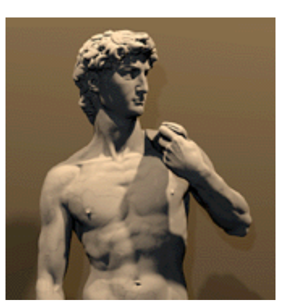
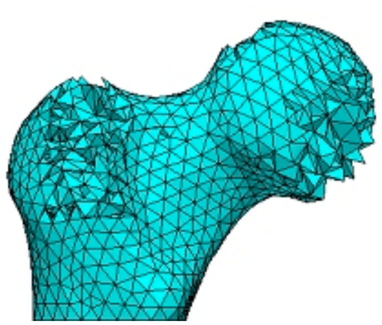
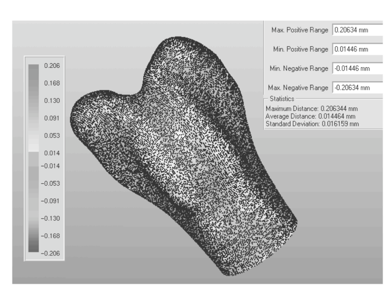
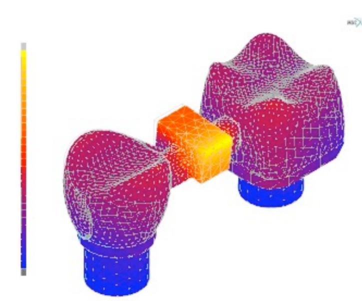
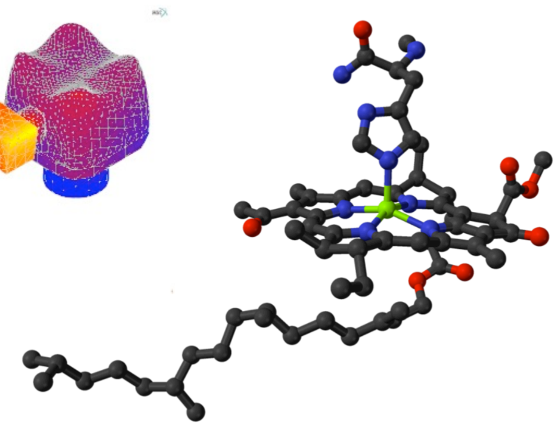
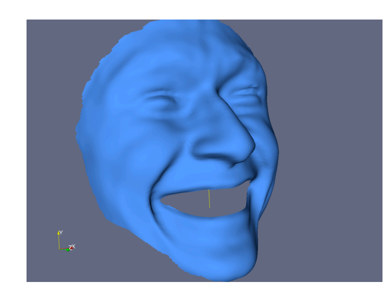
The Problem of Shape/Object Matching

- databases of *objects*
- objects can be many things:
  - proteins
  - molecules
  - 2D objects (imaging)
  - 3D shapes: as obtained via a 3D scanner
  - 3D shapes: modeled with CAD software
  - 3D shapes: coming from design of bone protheses
  - text documents
  - more complicated structures present
    in datasets (things you can't visualize)



3D objects: examples

- cultural heritage (Michelangelo project: `http://www-graphics.stanford.edu/projects/mich/`)
- search of parts in a factory of, say, cars
- face recognition: the face of an individual is a 3D shape...
- proteins: the *shape* of a protein reflects its function.. protein data bank: `http://www.rcsb.org`

Typical situation: classification

- assume you have database $\mathcal{D}$ of objects.
- assume $\mathcal{D}$ is composed by several objects, and that each of these objects belongs to one of n classes $C_1, \ldots, C_n$.
- imagine you are given a new object o, not in your database, and you are asked to determine whether o belongs to one of the classes. If yes, you also need to point to the class.
- One simple procedure is to say that you will assign object o the class of the *closest* object in $\mathcal{D}$:

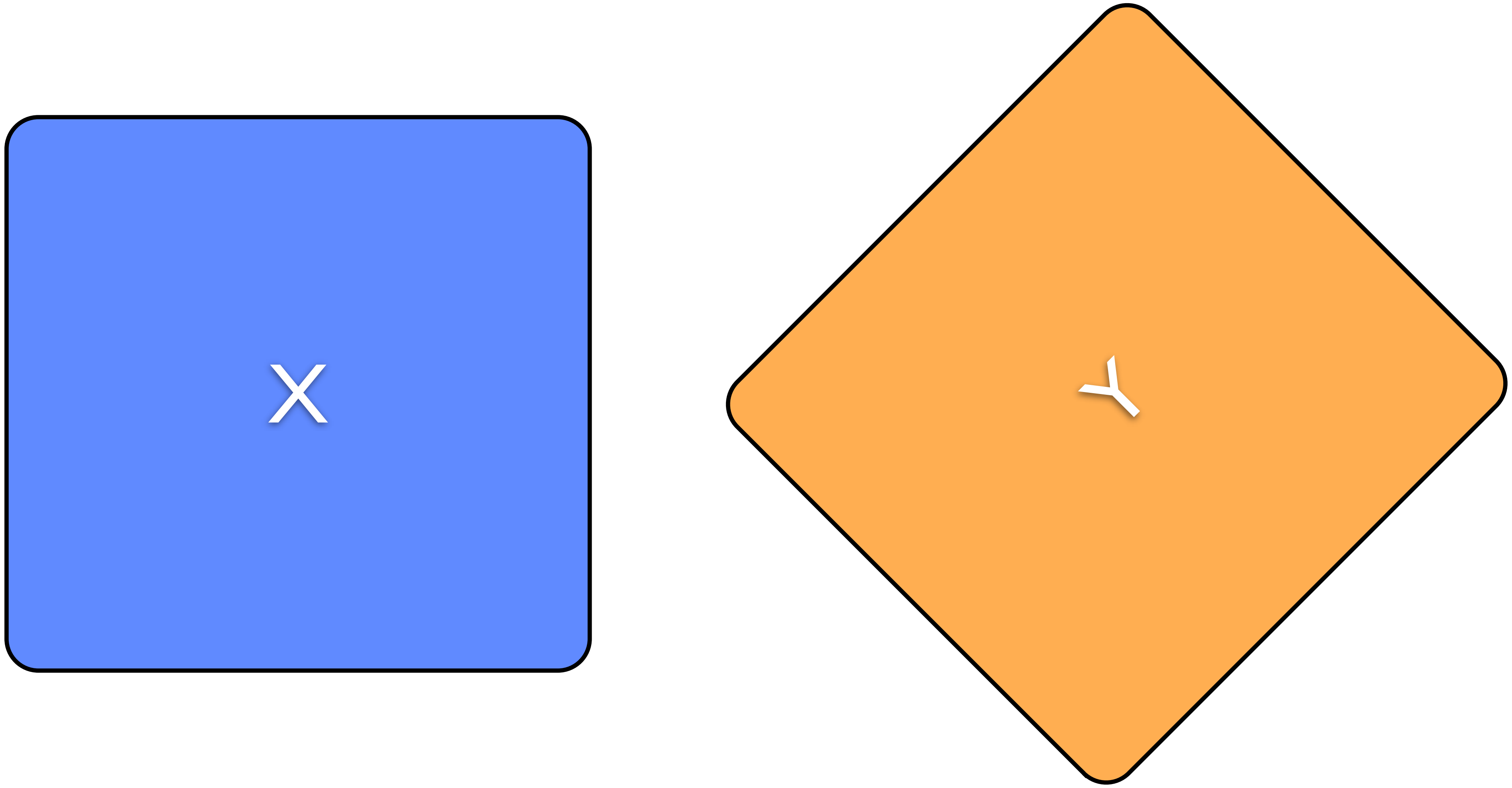
$$\text{class}(o) = \text{class}(z)$$

$$\text{where } z \in \mathcal{D} \text{ minimizes } \mathbf{dist}(o, z)$$

- in order to do this, one first needs to define a notion **dist** of *distance* or *dis-similarity between objects.*

Another important point: invariances

Are these two objects the same?



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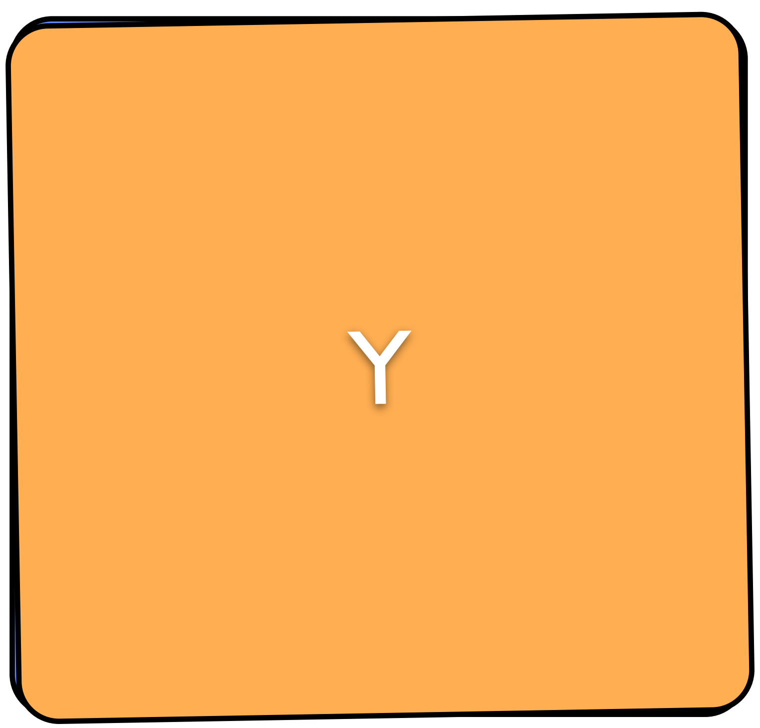
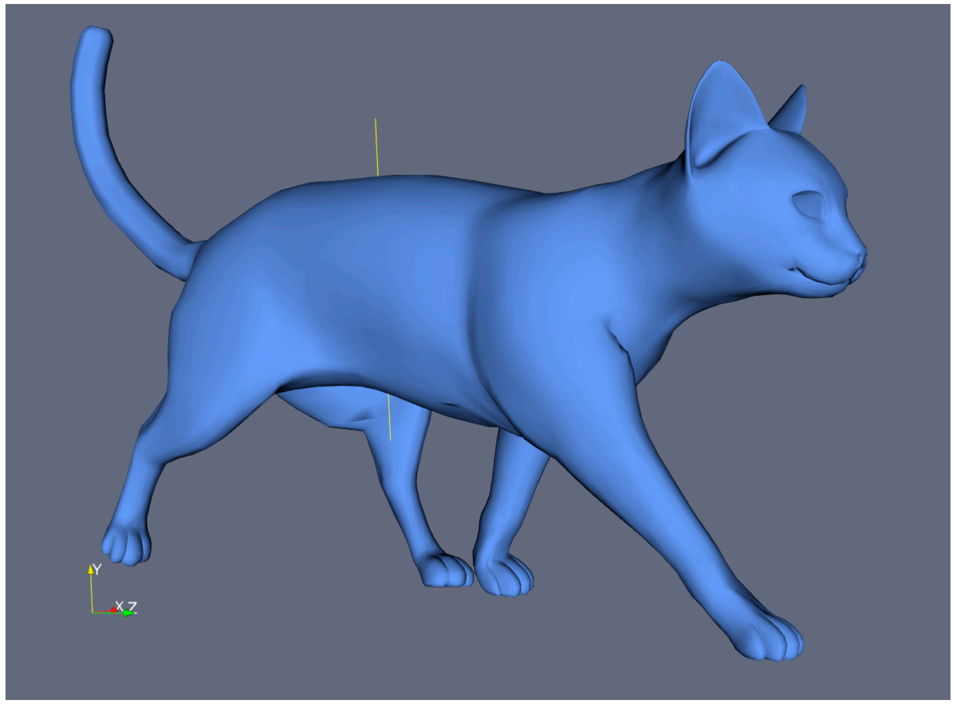
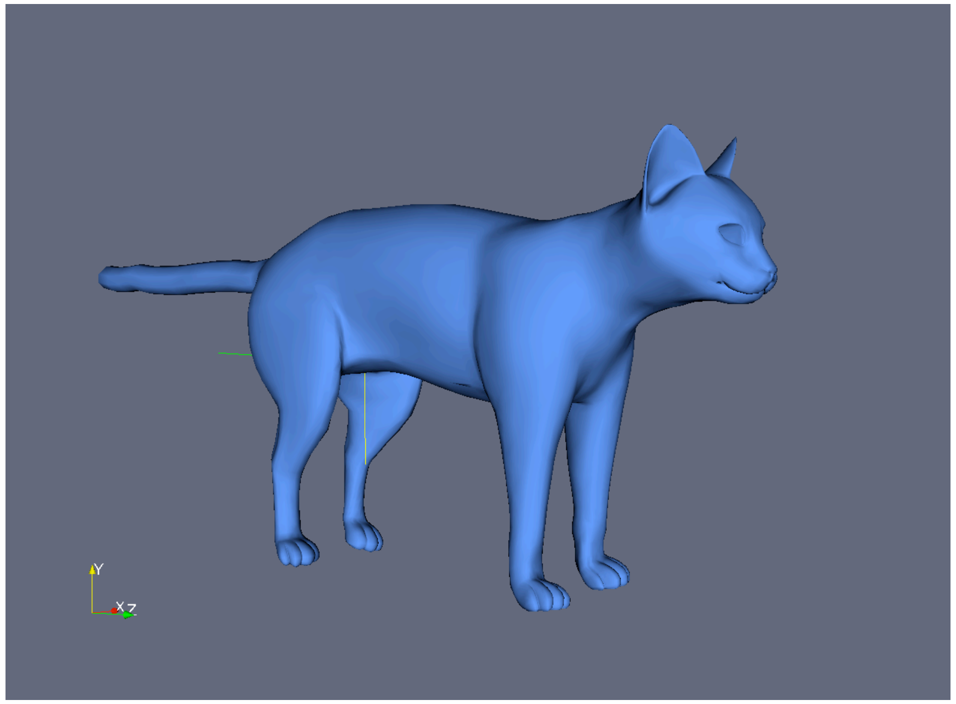


this is called invariance to *rigid transformations*

Another important points: invariances

what about these two?

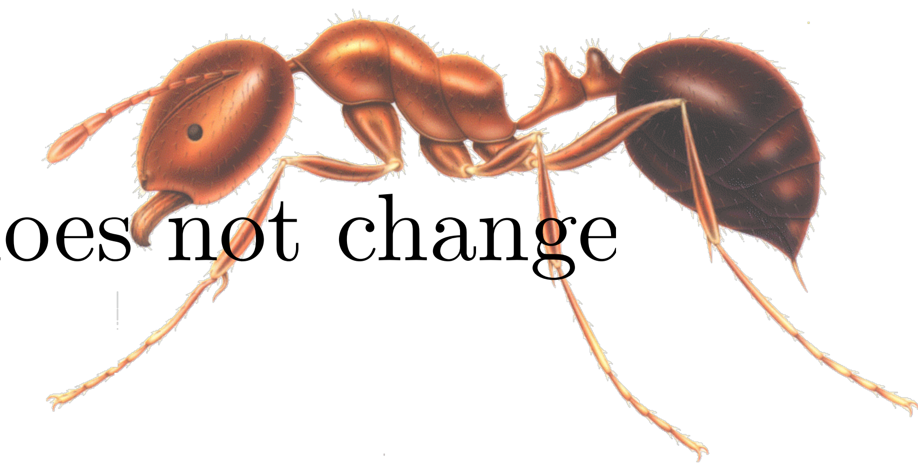


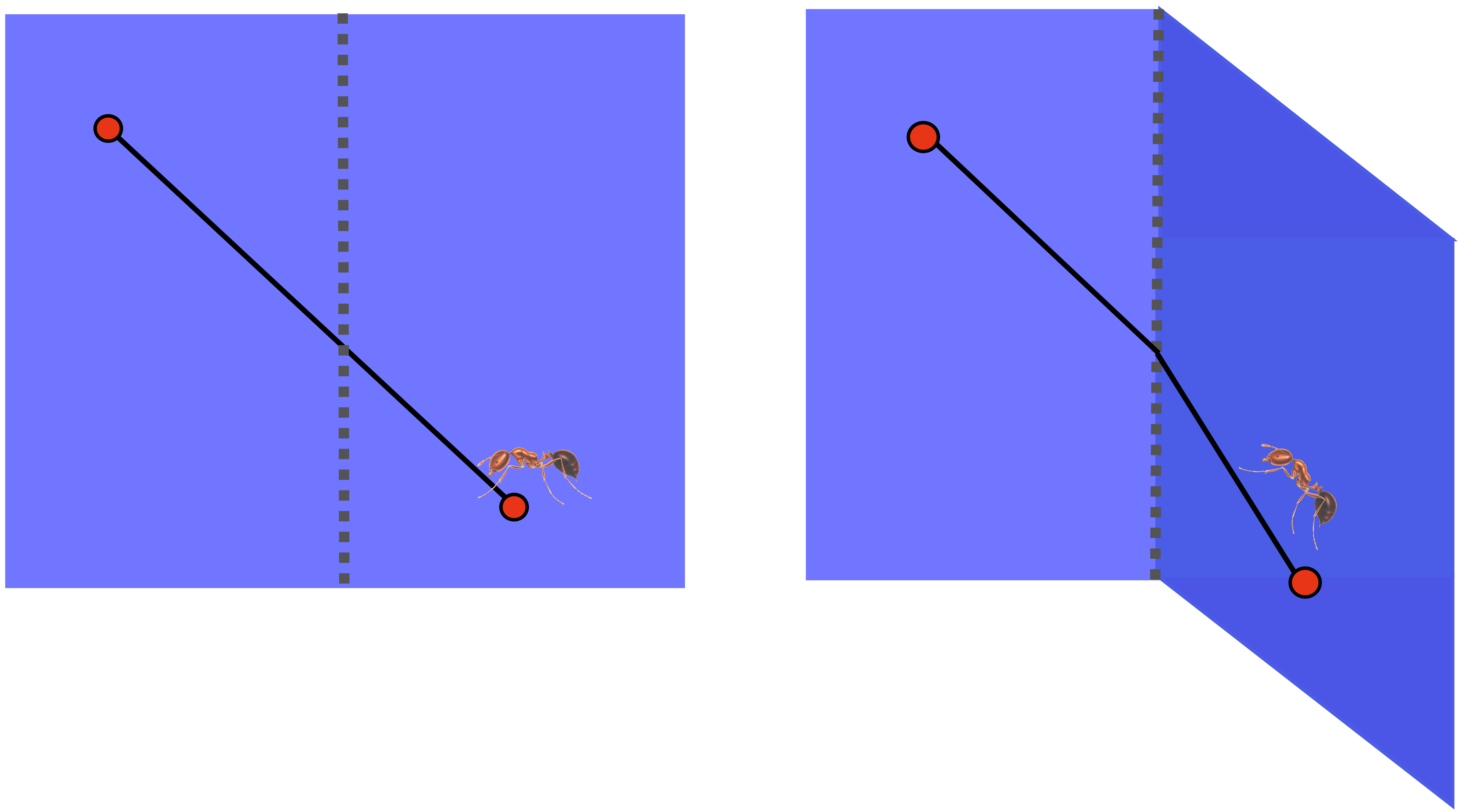


roughly speaking, this corresponds to invariance to *bending transformations*..

Bending transformations

the distance, as measured by an ant, does not change





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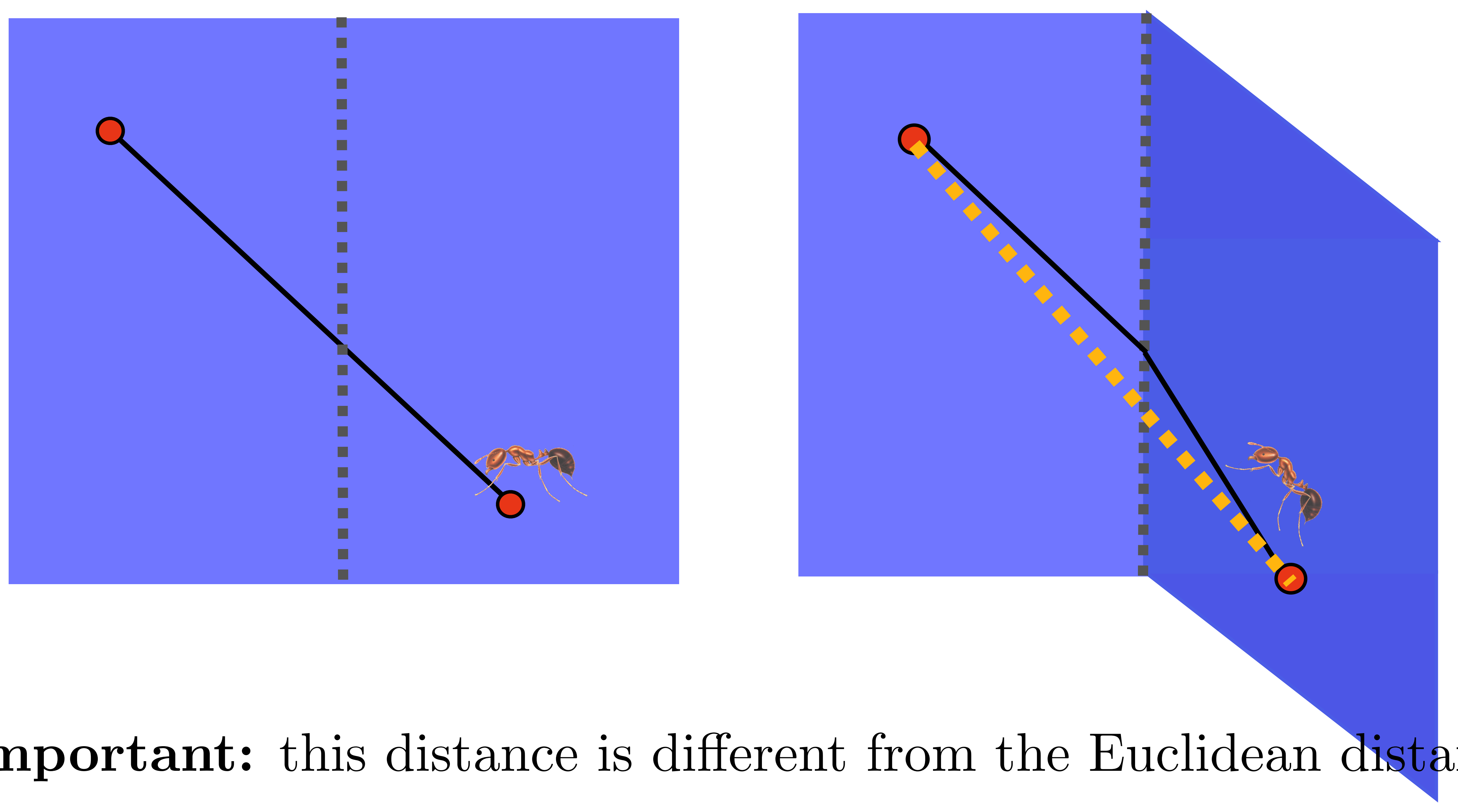
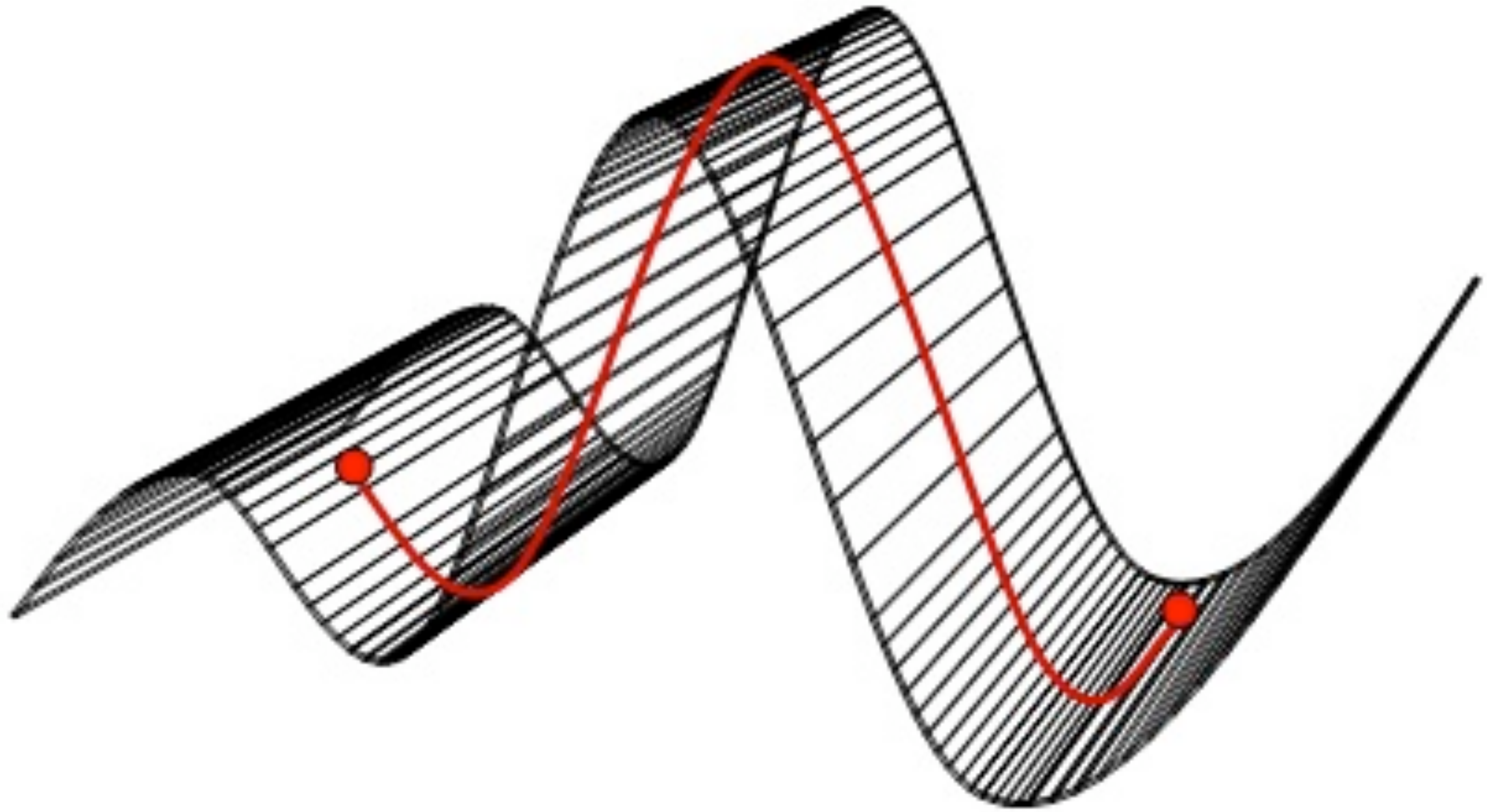
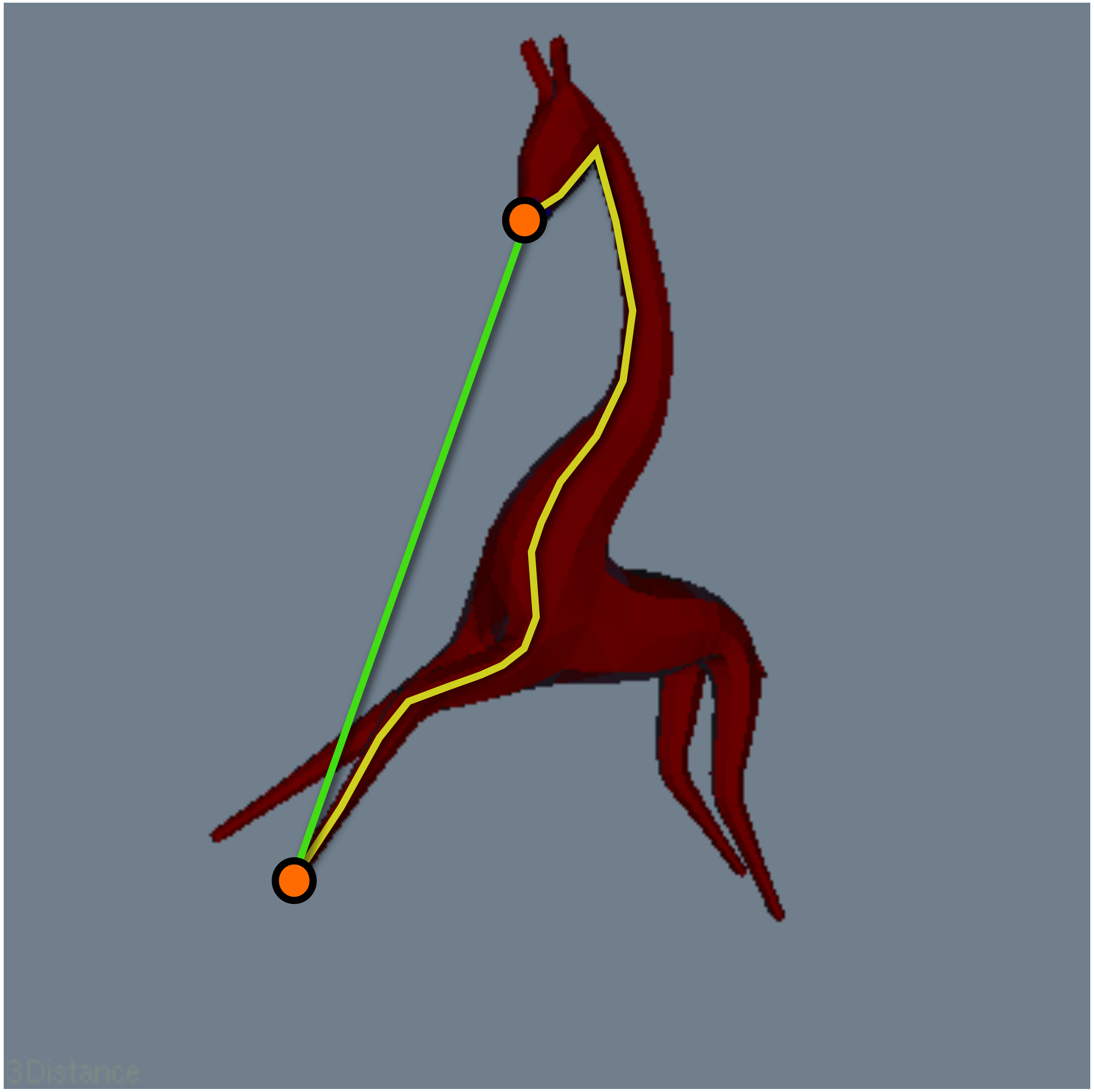


Important: this distance is different from the Euclidean distance!!



Geodesic distance vs Euclidean distance

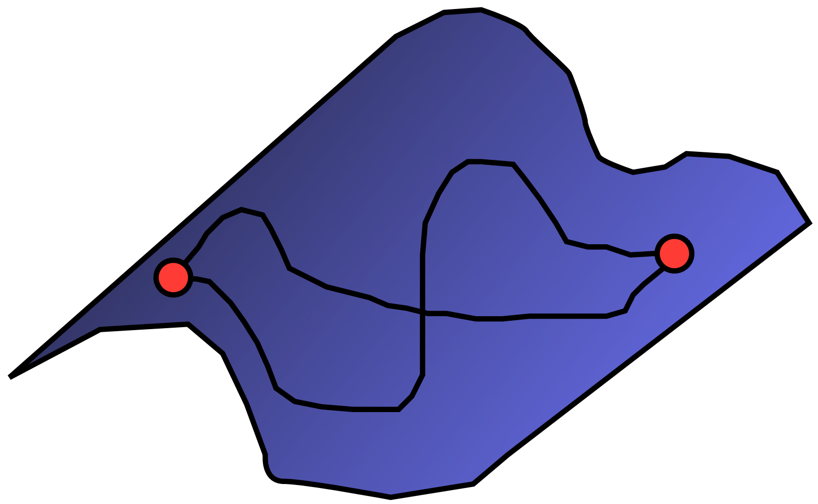


Geodesic/intrinsic distance

Let S be a (compact, path connected) a surface in $\mathbb{R}^3$. Given two points $x, y \in S$ let $\Gamma[x, y] := \{\gamma : [0, 1] \to S\}$ s.t. $\gamma(0) = x$ and $\gamma(1) = y$. For each Lipschitz curve γ let $\mathbf{L}(\gamma) := \int_0^1 \|\dot{\gamma}(t)\| \, dt$.

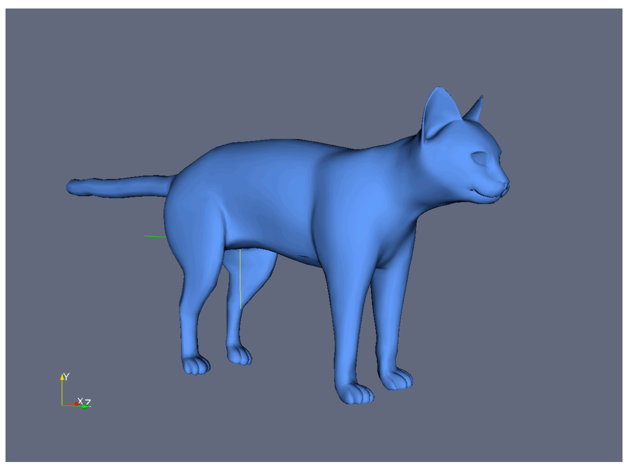
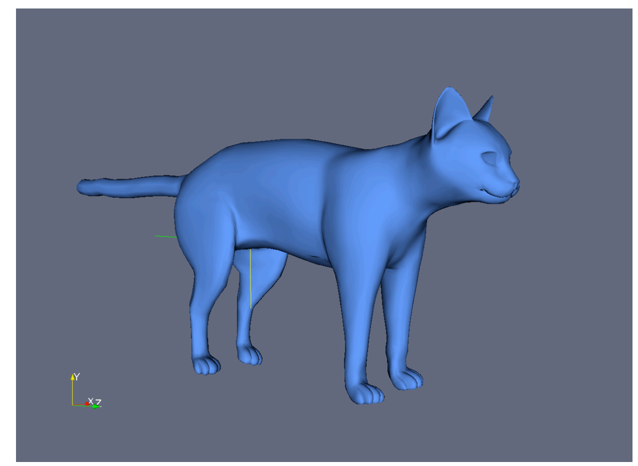
Then, let

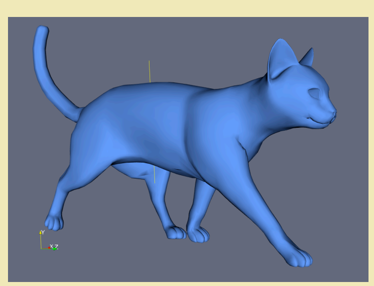
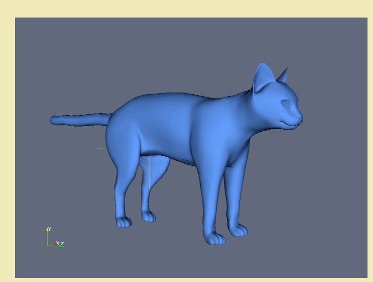
$$d_S(x, y) = \inf_{\gamma \in \Gamma[x,y]} \mathbf{L}(\gamma)$$



invariances...

The measure of dis-similarity **dist** must capture the type of invariance you want to encode in your classification system.

 =  ?

dist( , ) = 0 ?

Background concepts

• **Metric Space**. A metric space is a pair (X, d) where X is a set and $d : X \times X \to \mathbb{R}^+$, called the metric, s.t.

1. For all $x, y, z \in X$, $d(x, y) \leq d(x, z) + d(z, y)$.
2. For all $x, y \in X$, $d(x, y) = d(y, x)$.
3. $d(x, y) = 0$ if and only if $x = y$.

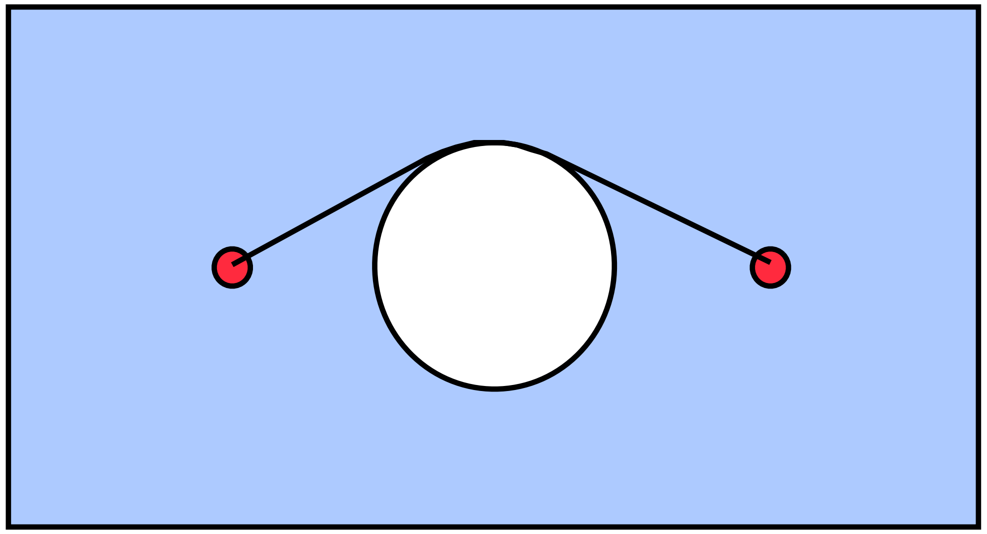
Remark 1. *One example is $\mathbb{R}^d$ with the Euclidean metric. Spheres S^n endowed with the spherical metric provide another example.*

• **Induced intrinsic metric [BBI, §2.3.3]** Given a (path connected) compact metric space (X, d) we consider a new metric on X, denoted by $\mathcal{L}(d)$ given by the following construction

$$\mathcal{L}(d)(x, y) = \inf_{\gamma \in \Gamma[x,y]} \mathbf{L}(\gamma).$$

This new metric, is called the induced intrinsic metric, or intrinsic metric for short. We will sometimes call it geodesic metric too.

- Compare with idea behind *Dijkstra* algorithm on Graphs.
- $\mathcal{L}(d) \neq d$ in general...think of case of the plane without a circle:



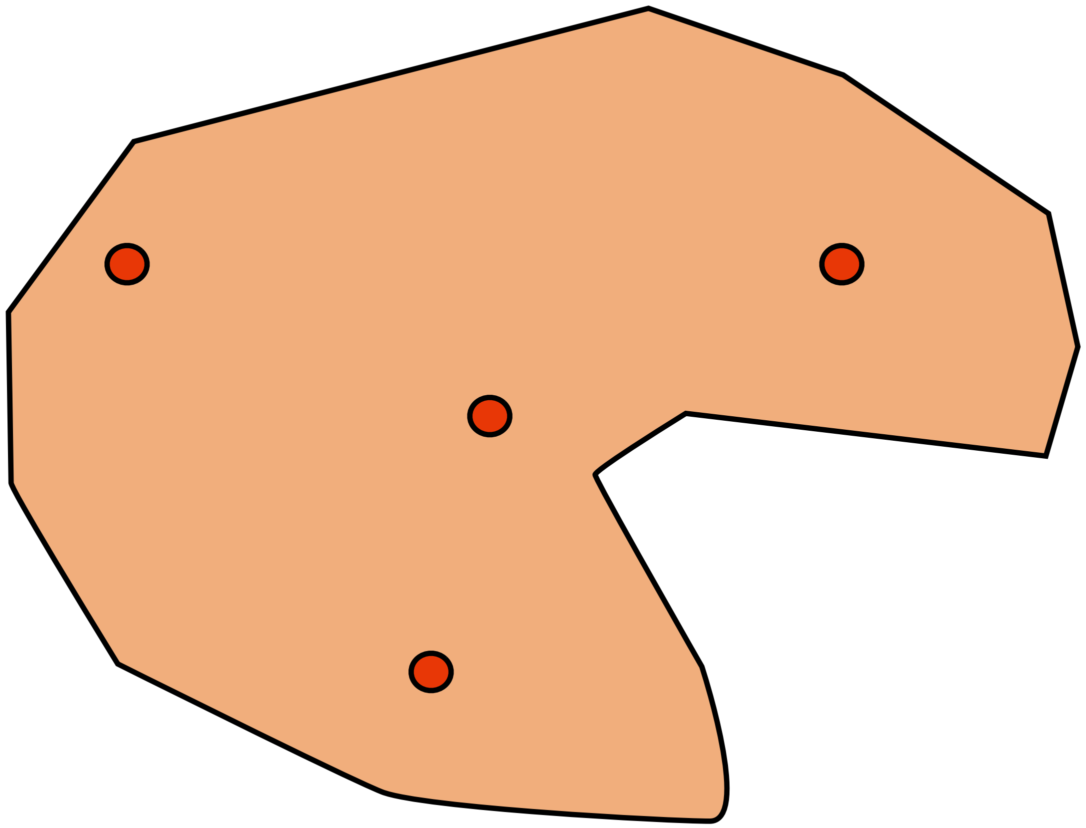
- ε**-net**. Given a metric space (X, d) and $A \subset X$ we say that A is an ε-net of X if for all $x \in X$ there exists $a \in A$ s.t. $d(x, a) \leq \varepsilon$.

- **Ball**

  - An *open* ball of radius r centered at $x \in X$ is the set $B_X(x, r) = \{x' \in X \mid d(x, x') < r\}$.

  - A *closed* ball of radius r centered at $x \in X$ is the set $B_X(x, r) = \{x' \in X \mid d(x, x') \leq r\}$.

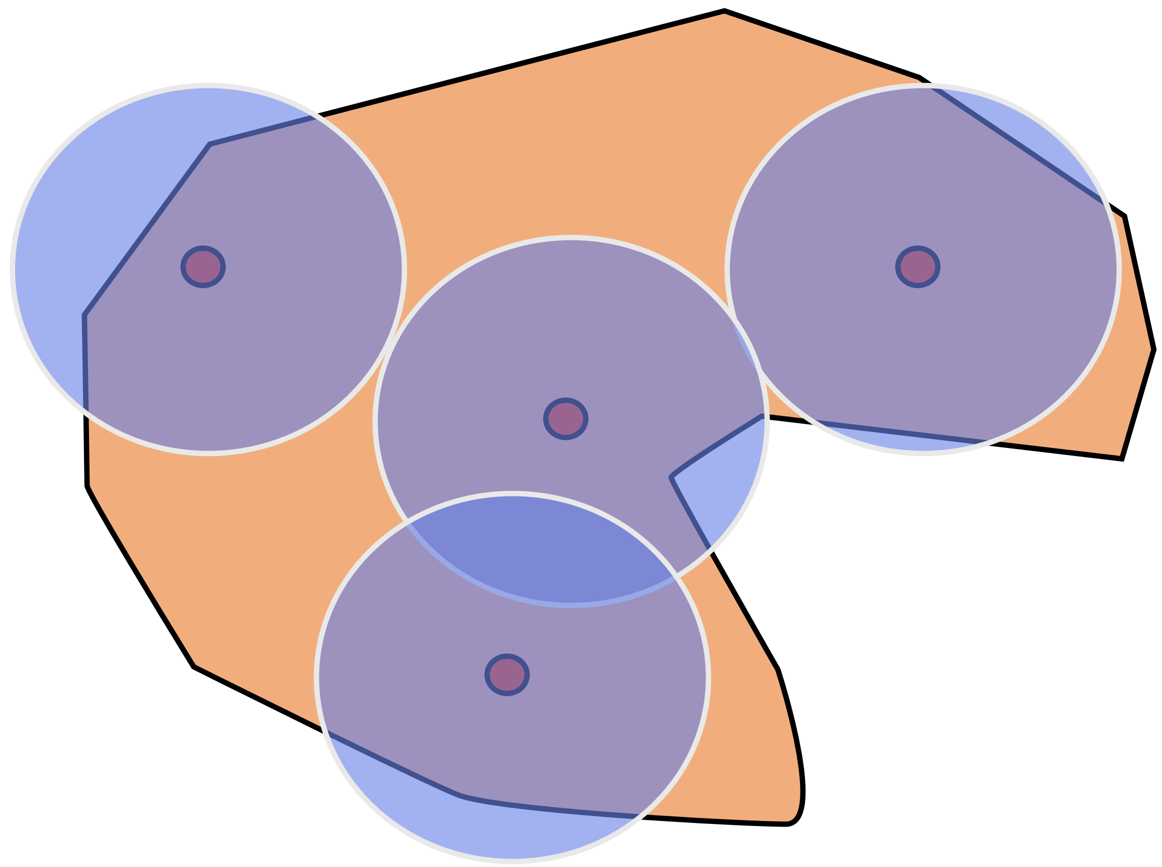
(X, d)



A is composed by the 4 points in red

$A^{\varepsilon} = \cup_{a \in A} B_X(a, \varepsilon)$

(X, d)



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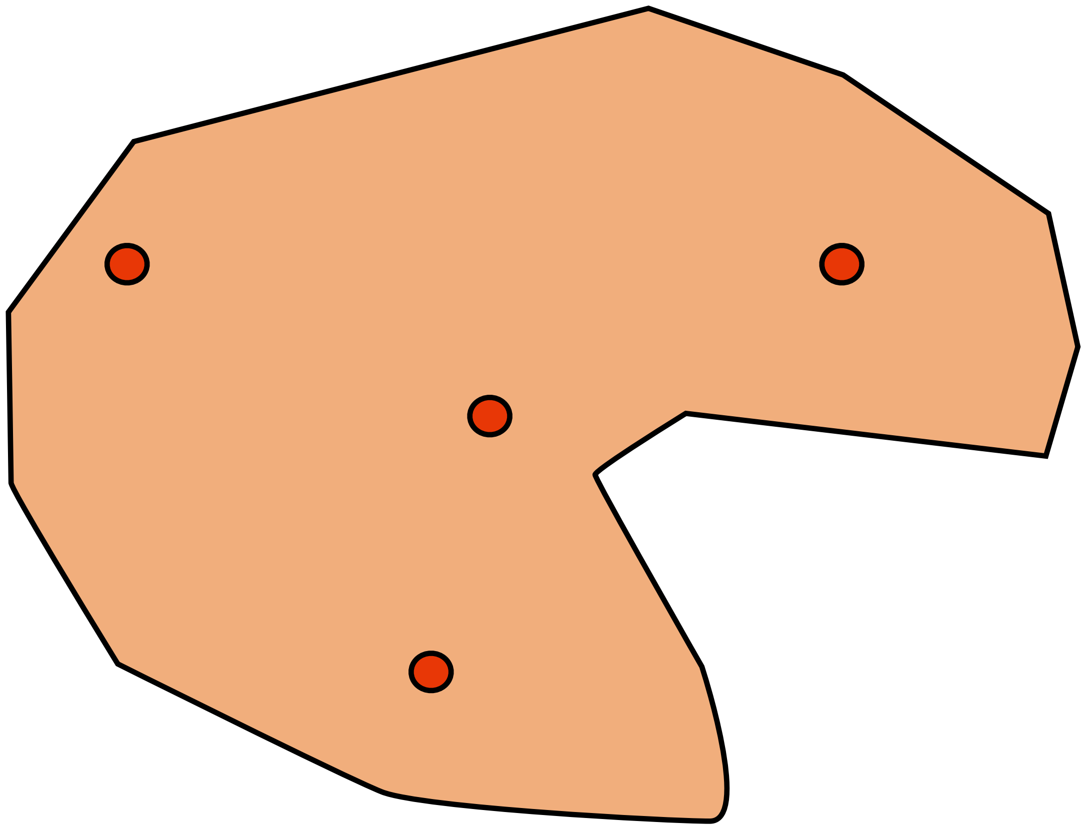

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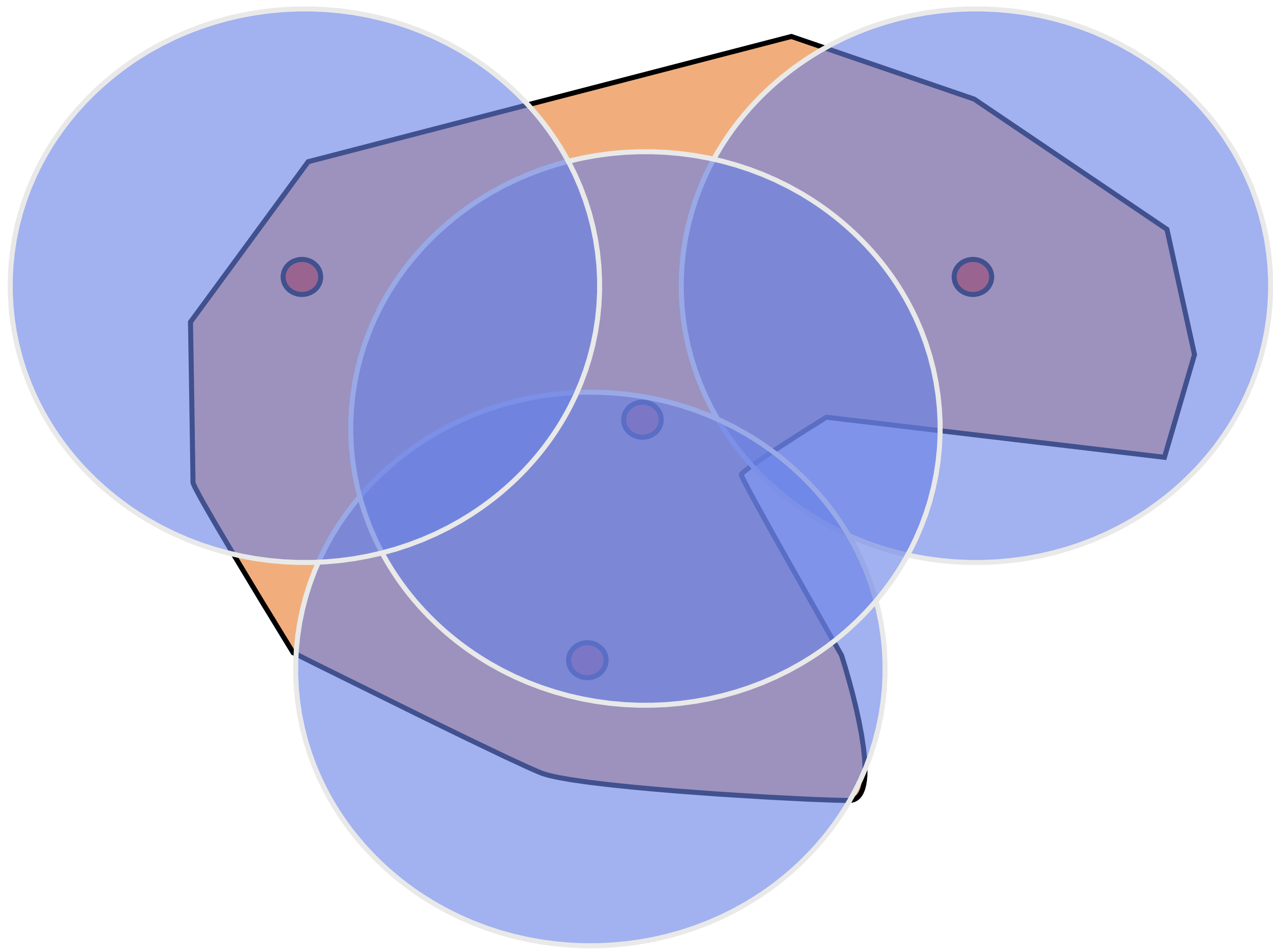

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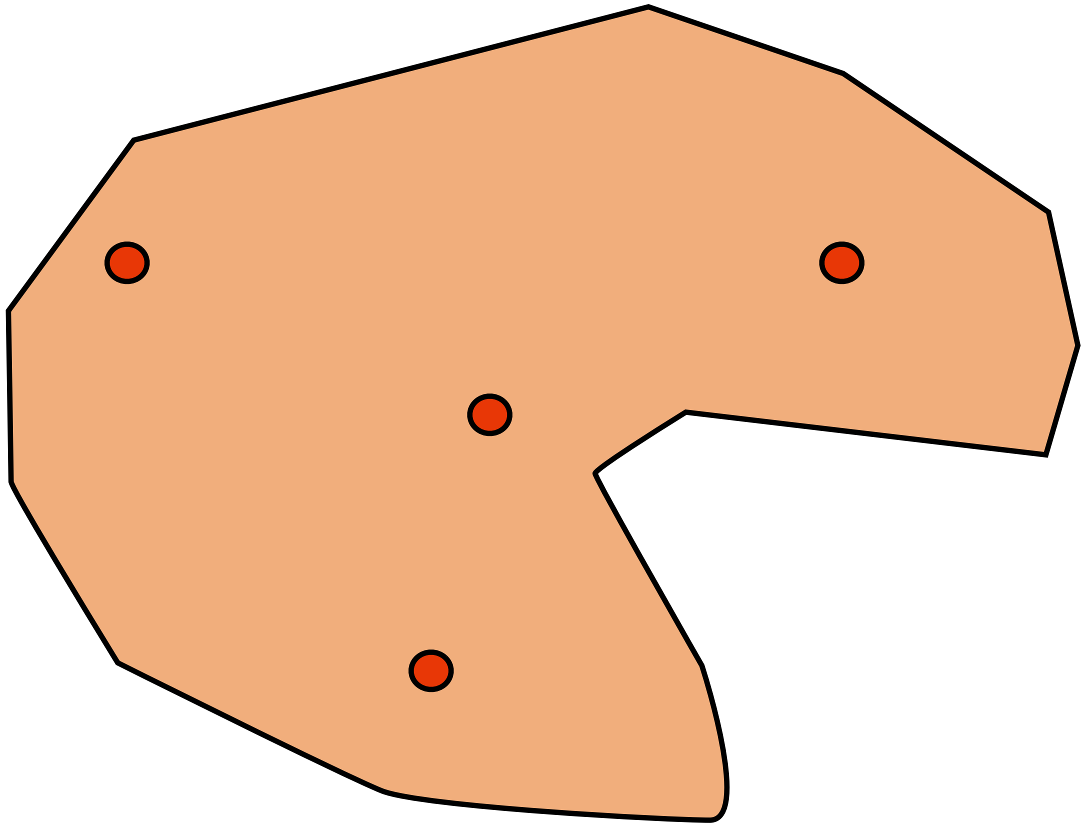

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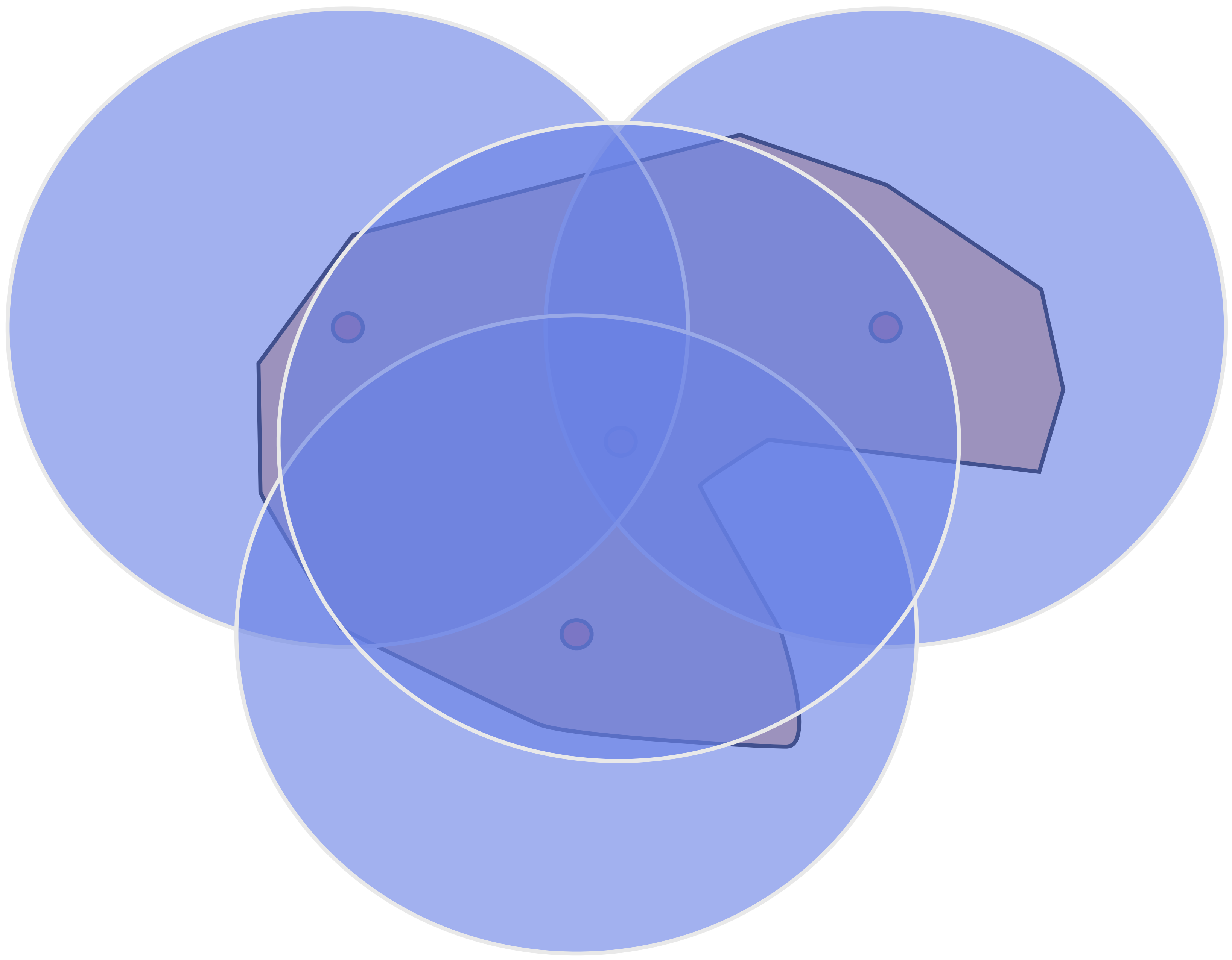


A is composed by the 4 points in red

$A^{\varepsilon} = \cup_{a \in A} B_X(a, \varepsilon)$

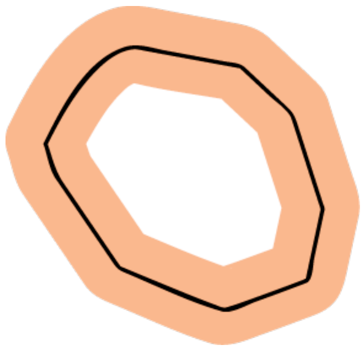
Hence, if $X \subset A^{\varepsilon}$, then A is an ε-net for X.

a couple of facts: Let (X, d) be a *compact* metric space

- Given $A \subset X$ there exists finite $\varepsilon > 0$ s.t. $X \subset A^{\varepsilon}$.
- Given $\varepsilon > 0$ there exists finite $A \subset X$ s.t. $X \subset A^{\varepsilon}$.

Note: ε-nets are also often referred to as ε-coverings.

this brings us to the Hausdorff distance between subsets of a metric space..



Fix a metric space (X, d).The intuition is that an object is a collection or a set of points in X.

Given a compact metric space (X, d), I will denote by $\mathcal{C}(X)$ the set of all compact subsets of X. I will say that $\mathcal{C}(X)$ is the collection of <u>objects</u> that live in X.

The leitmotiv of this class is that we will be looking at the set of all objects in a fixed ambient space, as a metric space itself!! This means that we will need to specify a way of measuring distance between objects. We do this in the next slide:

$$(X, d) \mapsto (\mathcal{C}(X), \mathbf{dist}).$$

- **Hausdorff distance**. For (compact) subsets A, B of a (compact) metric space (Z, d), the *Hausdorff distance* between them, $d_{\mathcal{H}}^{Z}(A, B)$, is defined to be the infimal $\varepsilon > 0$ s.t.

$$A \subset B^{\varepsilon} \text{ and } B \subset A^{\varepsilon}$$

Equivalently,

$$d_{\mathcal{H}}^{Z}(A, B) = \max(\max_{b \in B} \min_{a \in A} d(a, b), \max_{a \in A} \min_{b \in B} d(a, b)).$$

For a subset A of a metric space (X, d) we will use the notation $d(x, A) := \inf_{a \in A} d(x, a)$.

Theorem ([**BBI**], Proposition 7.7.3)**.** *The Hausdorff distance is a* metric *on the set of all objects (i.e.* compact *subsets) of* X, $\mathcal{C}(X)$.

correspondences

Definition [Correspondences]

For sets A and B, a subset $R \subset A \times B$ is a *correspondence* (between A and B) if and and only if

- $\forall\ a \in A$, there exists $b \in B$ s.t. $(a, b) \in R$
- $\forall\ b \in B$, there exists $a \in A$ s.t. $(a, b) \in R$

Let $\mathcal{R}(A, B)$ denote the set of all possible correspondences between sets A and B.

Remark. *Note that $\mathcal{R}(A, B) \neq \emptyset$. Indeed, $A \times B$ is always in $\mathcal{R}(A, B)$.*

correspondences

Note that when A and B are finite, $R \in \mathcal{R}(A, B)$ can be represented by a matrix $((r_{a,b})) \in \{0,1\}^{n_A \times n_B}$ s.t.

$$\sum_{a \in A} r_{ab} \geq 1 \ \ \forall b \in B$$

$$\sum_{b \in B} r_{ab} \geq 1 \ \ \forall a \in A$$

$$\begin{array}{cc} & B \\ A & \begin{array}{|c|c|c|c|c|c|c|} \hline 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ \hline 1 & 1 & 0 & 1 & 0 & 1 & 1 \\ \hline 1 & 0 & 1 & 0 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ \hline \end{array} \end{array}$$

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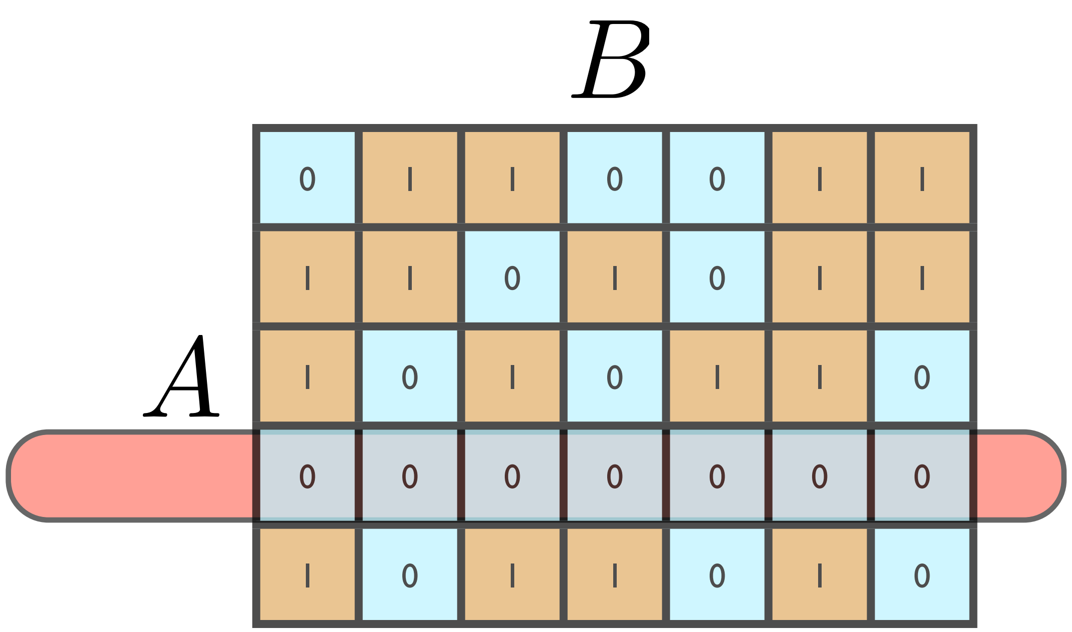

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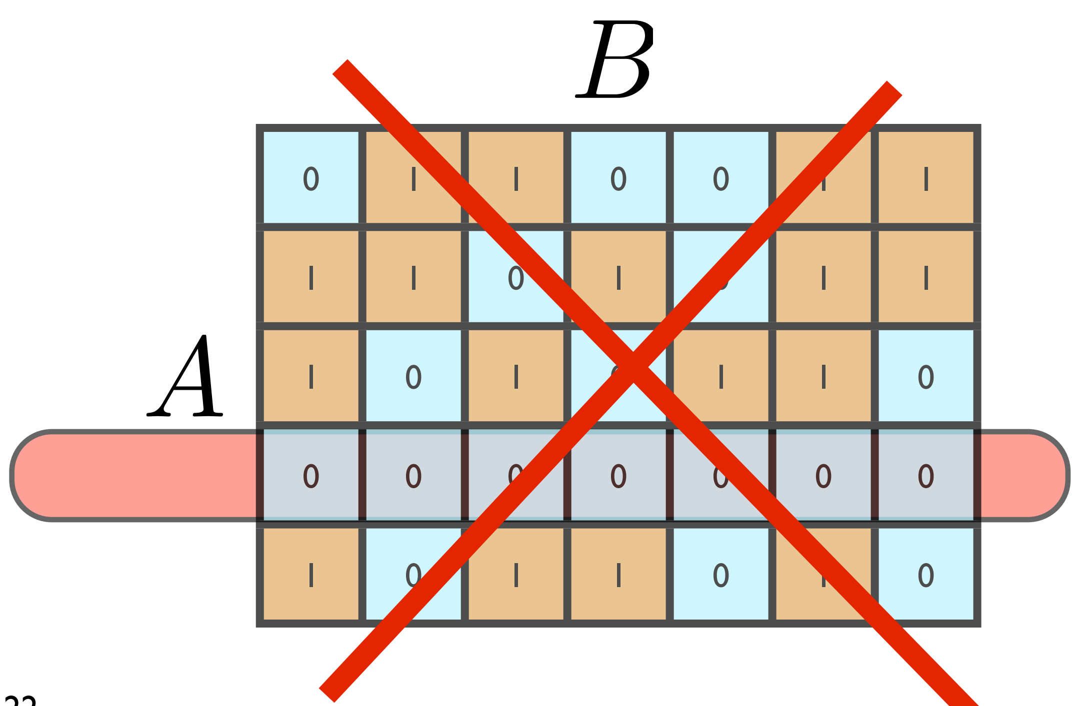

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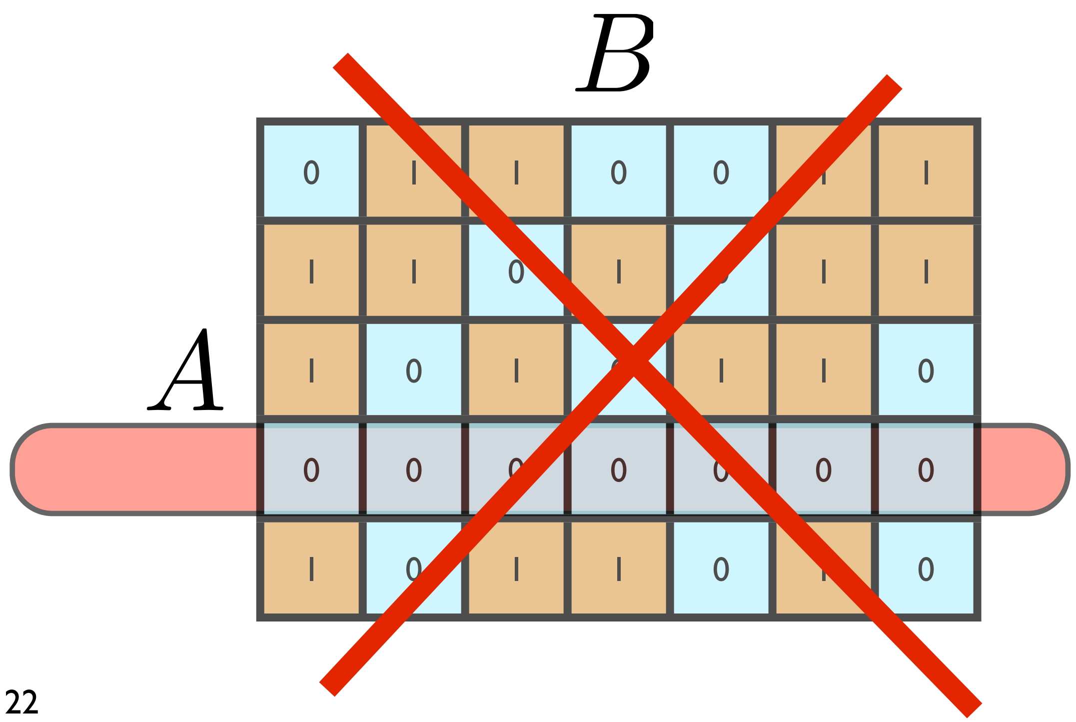

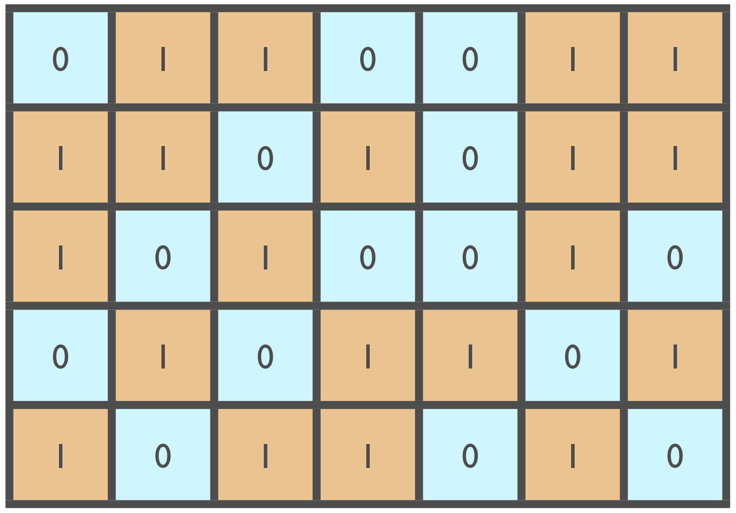

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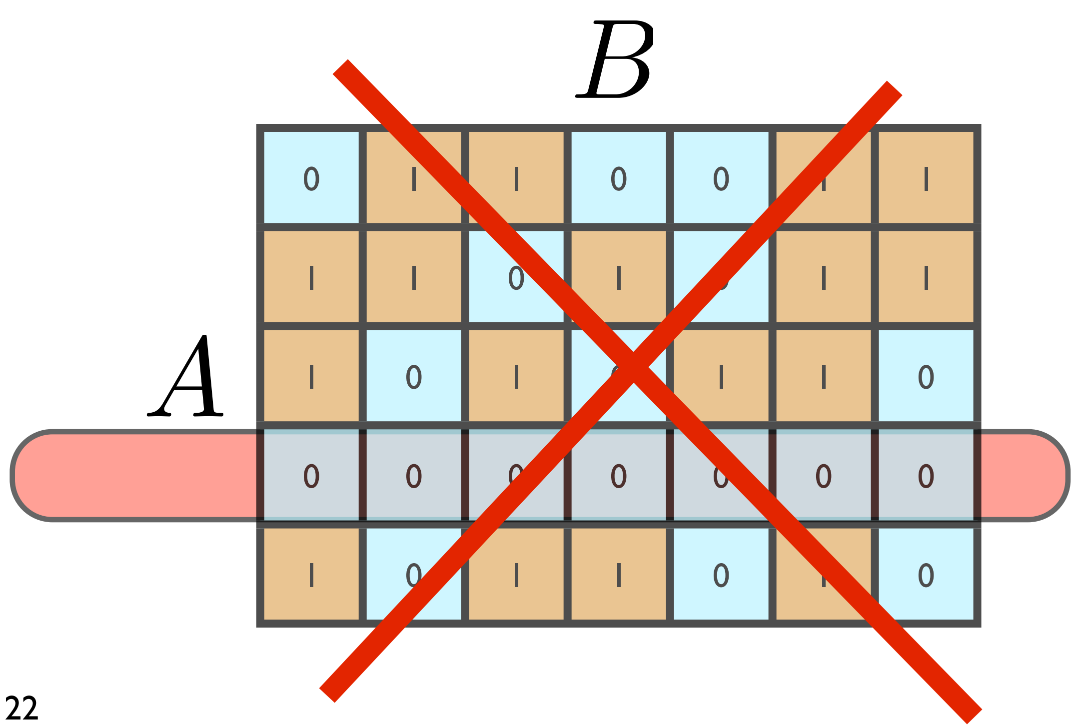
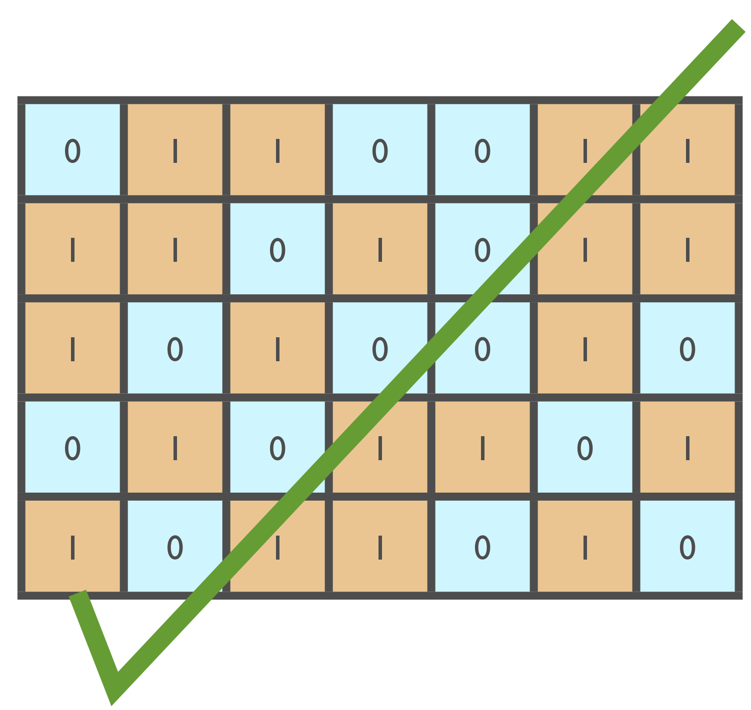




Examples and remarks

The proof of the results below is an exercise.

- If $A = \{a_1, \ldots, a_n\}$ and $B = \{p\}$, then, $\mathcal{R}(A, B) = \{R\}$, where $R = \{(x_i, p),\, 1 \leq i \leq n\}$..

- If $A = \{a_1, \ldots, a_n\}$ and $B = \{b_1, \ldots, b_n\}$, then for all $\pi \in \Pi_n$ (permutations of $\{1, \ldots, n\}$), $\{(a_i, b_{\pi_i}),\, 1 \leq i \leq n\} \in \mathcal{R}(A, B)$. Hence, correspondences include bijections (when these exist).

- **Composition of correspondences.** If A, B, C are sets and $R \in \mathcal{R}(A, B)$ and $S \in \mathcal{R}(B, C)$, then

  $$T := \{(a, c) |\, \exists b \in B \,\text{s.t.}\, (a, b) \in R \,\text{and}\, (b, c) \in S\}$$

  belongs to $\mathcal{R}(A, C)$.

- Let $f : A \to B$ and $g : B \to A$ be given. Then,

  $$\{(a, f(a)),\, a \in A\} \cup \{\, (g(b), b),\, b \in B\} \in \mathcal{R}(A, B).$$

Theorem (An important observation, **[M07]**). *Let (X,d) be a compact metric space. Then, for all compact $A, B \subset X$,*

$$d_{\mathcal{H}}^X(A,B) = \inf_{R \in \mathcal{R}(A,B)} \sup_{(a,b)\in R} d(a,b).$$

Proof. Exercise. $\square$

Remark. *We will use the following notation: for a function $f : Z \to \mathbb{R}$ and $C \subset Z$, we let*

$$\|f\|_{L^\infty(C)} := \sup_{z \in C} |f(c)|.$$

Remark. *Then, we can write in a somewhat abbreviated way that will be used for reasoning about potential candidates for* **dist***,*

$$d_{\mathcal{H}}^X(A,B) = \inf_{R \in \mathcal{R}(A,B)} \|d\|_{L^\infty(R)}.$$

Exercise. *Using the expression for the H-distance above and the remark on composition of correspondences prove the triangle inequality for the H-distance.*

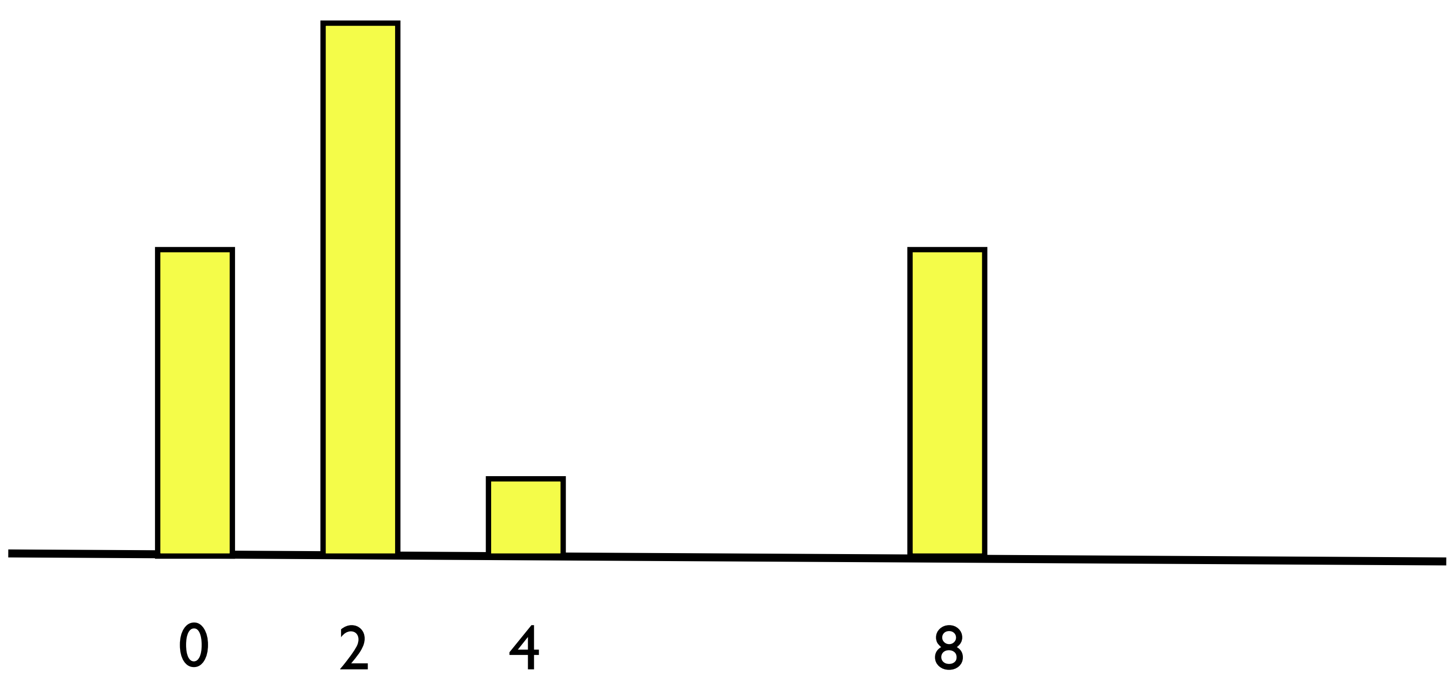
- **Probability Measures.** Consider a finite set $A = \{a_1, \ldots, a_n\}$. A set of *weights*, $W = \{w_1, \ldots, w_n\}$ on A is called a *probability measure* on A if $w_i \geq 0$ and $\sum_i w_1 = 1$.

Probability measures can be interpreted as a way of assigning (relative) importance to different points.

There is a more general definition that we do not need (today). But you should become familiar with it for general culture, see [**BBI, Def. 1.7.1**].

• **Support of a measure.** Given a metric space (X, d) and a probability measure ν on X, the *support* of ν consists of the points of X with non-zero *mass*. We use the notation $\mathrm{supp}(\nu)$ for the support of a probability measure ν on X.

Example. *Consider for example the case of* $X = \mathbb{R}$ *with the usual metric. Let* ν *be the probability measure on the real line that assigns mass* $1/4$, $5/12$, $1/12$ *and* $1/4$ *to points* 0, 2, 4 *and* 8, *respectively. Then, there is no mass anywhere else and* $supp(\nu) = \{0, 2, 4, 8\}$.



correspondences and measure couplings

Let A and B be compact subsets of the compact metric space (X, d) and μ_A and μ_B be **probability measures** supported in A and B respectively.

Definition [Measure coupling] Is a probability measure μ on $A \times B$ s.t. (in the finite case this means $((\mu_{a,b})) \in [0,1]^{n_A \times n_B}$, i.e. μ is a *matrix*.)

- $\sum_{a \in A} \mu_{ab} = \mu_B(b) \;\; \forall b \in B$
- $\sum_{b \in B} \mu_{ab} = \mu_A(a) \;\; \forall a \in A$

Let $\mathcal{M}(\mu_A, \mu_B)$ be the set of all couplings of μ_A and μ_B.
Notice that in the finite case, $((\mu_{a,b}))$ must satisfy $n_A + n_B$ *linear* constraints.

Y

X

	0.30	0.30	0.40
0.25	0.25	0	0
0.25	0	0.15	0.10
0.25	0	0.1	0.15
0.25	0.05	0.05	0.15

Example. *In this example,*

$$supp(\mu) = \{(x_1, y_1), (x_2, y_2), (x_2, y_3), (x_3, y_2), (x_3, y_3), (x_4, y_1), (x_4, y_2), (x_4, y_3)\}.$$

Example. *Assume* $X = \{x_1, \ldots, x_n\}$ *and* $Y = \{p\}$, *together with an arbitrary* μ_X *supported on* X *and* μ_Y *s.t.* $\mu_Y(p) = 1$ *(all the mass is in* p*). Prove that*

$$\mathcal{M}(\mu_X, \mu_Y) = \{\mu_X\}.$$

(compare with exercise for correspondences)

Y

X

	0.30	0.30	0.40
0.25	0.25	0	0
0.25	0	0.15	0.10
0.25	0	0.1	0.15
0.25	0.05	0.05	0.15

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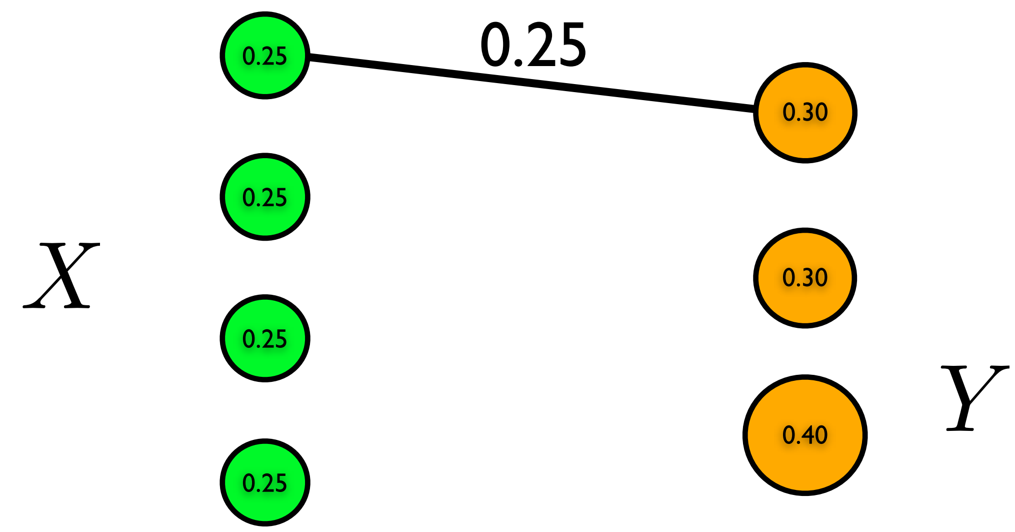

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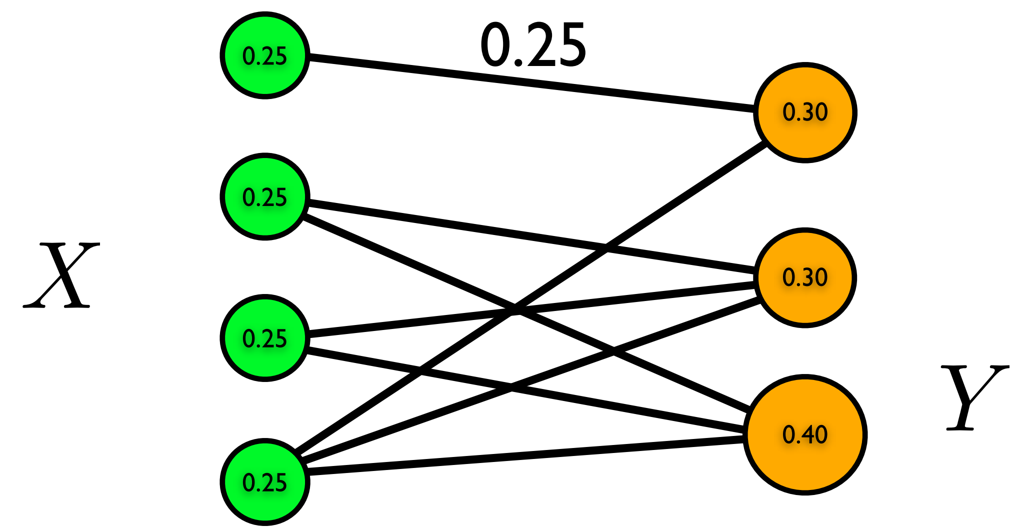

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(compare with exercise for correspondences)

• **Composition of measure couplings**. Can you guess what is the construction in this setting? Cf. with "composition of correspondences".

Remark. *You should gain some intuition about the duality between correspondences and measure couplings. Think about this on your own.*

• **Product measure**. Assume A and B are finite sets and μ_A and μ_B are probability measures on A and B, respectively. We define a probability measure on $A \times B$, called the *product measure* and denoted $\mu_A \otimes \mu_B$ s.t.

$$\mu_A \otimes \mu_B(a, b) = \mu_A(a) \times \mu_B(b).$$

Remark. *It is then clear that $\mathcal{M}(\mu_A, \mu_B) \neq \emptyset$ as (exercise!!)* $\mu_A \otimes \mu_B \in \mathcal{M}(\mu_X, \mu_Y)$.

Proposition ($\mu \leftrightarrow R$)**.** *Let A, B be sets.*

- *Given (A, μ_A) and (B, μ_B), and $\mu \in \mathcal{M}(\mu_A, \mu_B)$, then*

$$R(\mu) := supp(\mu) \in \mathcal{R}(A, B).$$

- *König's Lemma. [gives conditions for $R \to \mu$] [We don't need precise statement.]*

Proof. Omitted! □

Remark. *Let $f : X \to$ be a function and ν a probability measure on X. Then, for $p \geq 1$ the L^p norm of f w.r.t. to ν is (in the case of X finite)*

$$\|f\|_{L^p(\nu)} := \left(\int_X |f(x)|^p \nu(x) \right)^{1/p} = \left(\sum_{x \in X} \nu(x) |f(x)|^p \right)^{1/p}$$

Remark.

- *Correspondences and measure couplings provide two different ways of putting objects in correspondence. This is necessary whenever one tries to compare two objects.*

- *correspondence are* combinatorial gadgets. *They pairings they encode are* hard *as opposed to the* soft *or relaxed notion provided by measure couplings.*

- *Measure couplings are* continous *gadgets. As a general, imprecise rule, using them instead will lead to continuous optimization problems instead of combinatorial optimization problems. "CnOPs are easier to deal with than CbOPs ".*

Wasserstein distance

$$d_{\mathcal{H}}(A, B) = \inf_{R \in \mathcal{R}(A,B)} \|d\|_{L^\infty(R)}$$

$$\Downarrow \ (R \leftrightarrow \mu)$$

$$d_{\mathcal{W},\infty}(A, B) = \inf_{\mu \in \mathcal{M}(\mu_A,\mu_B)} \|d\|_{L^\infty(R(\mu))}$$

$$\Downarrow \ (L^\infty \leftrightarrow L^p)$$

$$d_{\mathcal{W},p}(A, B) = \inf_{\mu \in \mathcal{M}(\mu_A,\mu_B)} \|d\|_{L^p(A \times B,\mu)}$$

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Remark. *When A and B are finite, a more explicit expression for the W-distance is*

$$d_{\mathcal{W},p}^X(A,B) := \min_{\mu}\left(\sum_{a,b} d(a,b)^p\,\mu(a,b)\right)^{1/p}$$

where $\mu \in \mathcal{M}(\mu_A,\mu_B)$.

Remark. *Notice that computing the W-distance leads to solving an* ***LOP*** *with linear and bound constraints.*

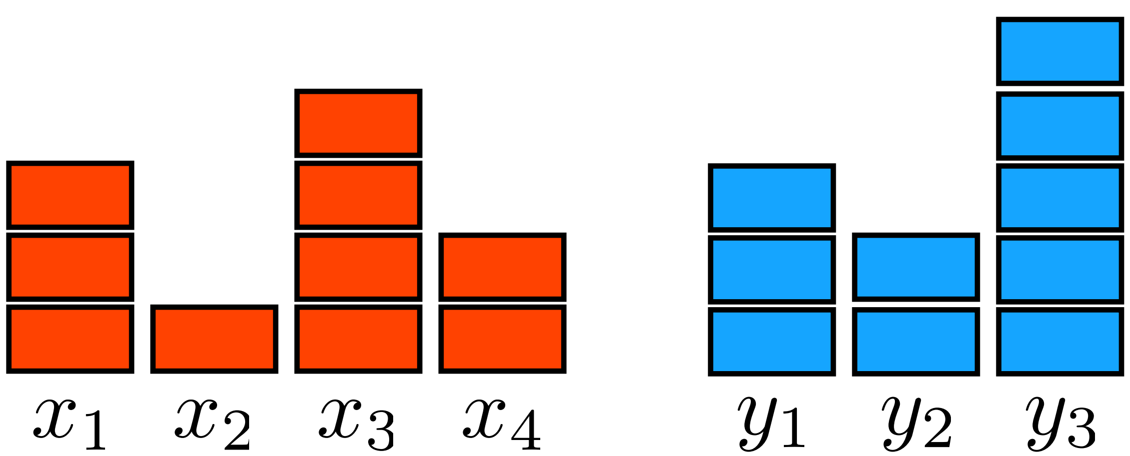
Remark. *We will see that $d_{\mathcal{H}}^X \leq d_{\mathcal{W},\infty}^X$. Can you prove this?*

Remark. • *The Wasserstein distance is a.k.a. EMD (Eart Mover's Distance) a.k.a. Kantorovich-Rubinstein.*

- *there is a very nice physical interpretation:* μ_A *represent a certain* source *profile of* n_A *bricks that must be moved from a certain location to another. The* target *profile at the destination, represented by* μ_B*, is such that the total number of bricks used is* equal *to* n_A.

- *The* cost *of moving a brick from location* x *to location* y *is* $d(x, y)$*, the horizontal distance between* x *and* y.

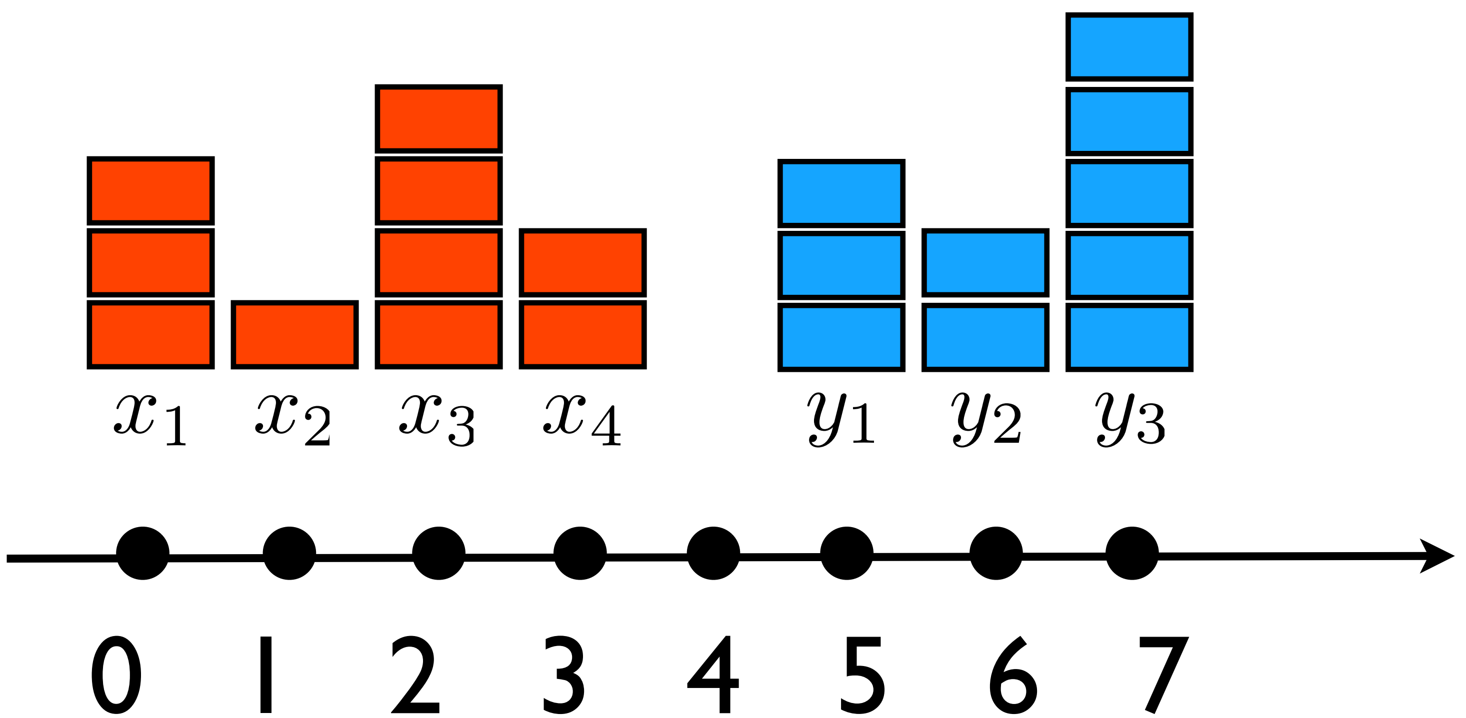
- *A measure coupling, in a first approximation, is a integer valued matrix that tells you how to distribute bricks in a source pile to the destination.*



	3	4	5
3			
1			
4			
2			

	3	2	5
3	**3**	0	0
1	0	0	**1**
4	0	0	**4**
2	0	**2**	0

$$\mathbf{cost}(\mu) = \sum_{x,y} d(x,y)\mu_{x,y}$$



$$\mathbf{cost}(\mu) = (3 \cdot 5 + 1 \cdot 6 + 4 \cdot 5 + 2 \cdot 3) = 47$$

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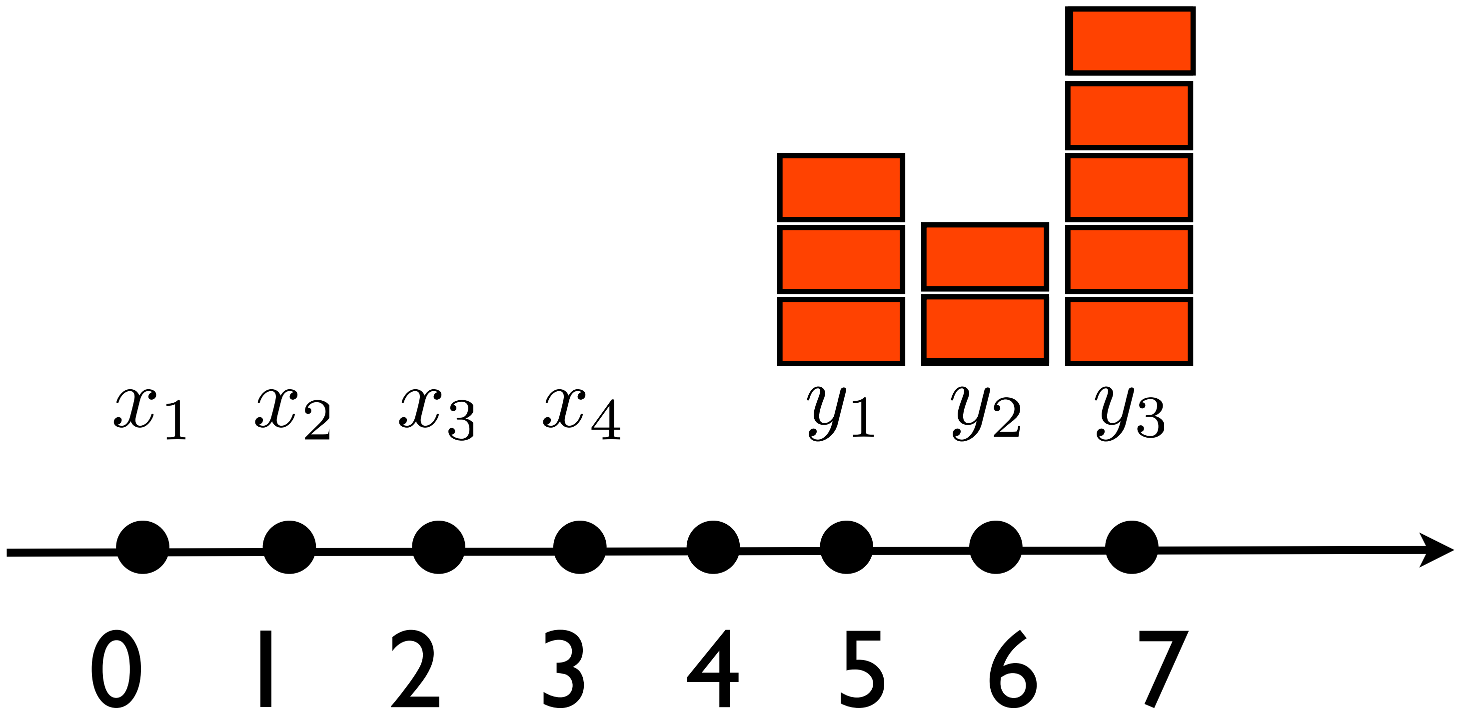


$$\mathbf{cost}(\mu) = (3 \cdot 5 + 1 \cdot 6 + 4 \cdot 5 + 2 \cdot 3) = 47$$

For a compact metric space (X, d) let

$$\mathcal{C}_w(X) := \{(A, \mu_A),\ A \in \mathcal{C}(X) \text{ and} \operatorname{supp}(\mu_A) = A\}.$$

This is the collection of all *weighted objects* in X.

Theorem ([**Villani**], see [**M07**])**.** *Let (X, d) be a compact metric space. The Wasserstein distance is a metric on $\mathcal{C}_w(X)$.*

• **Isometries**. Let (X, d_X) and (Y, d_Y) be two (compact) metric spaces. We say that a map $\phi : X \to Y$ is *distance preserving* if for all $x, x' \in X$,

$$\boxed{d_X(x, x') = d_Y(\phi(x), \phi(x')).}$$

If in addition, ϕ is *bijective*, then we say that ϕ is an *isometry*. We say that two metric spaces are isometric if there exists an isometry between them.

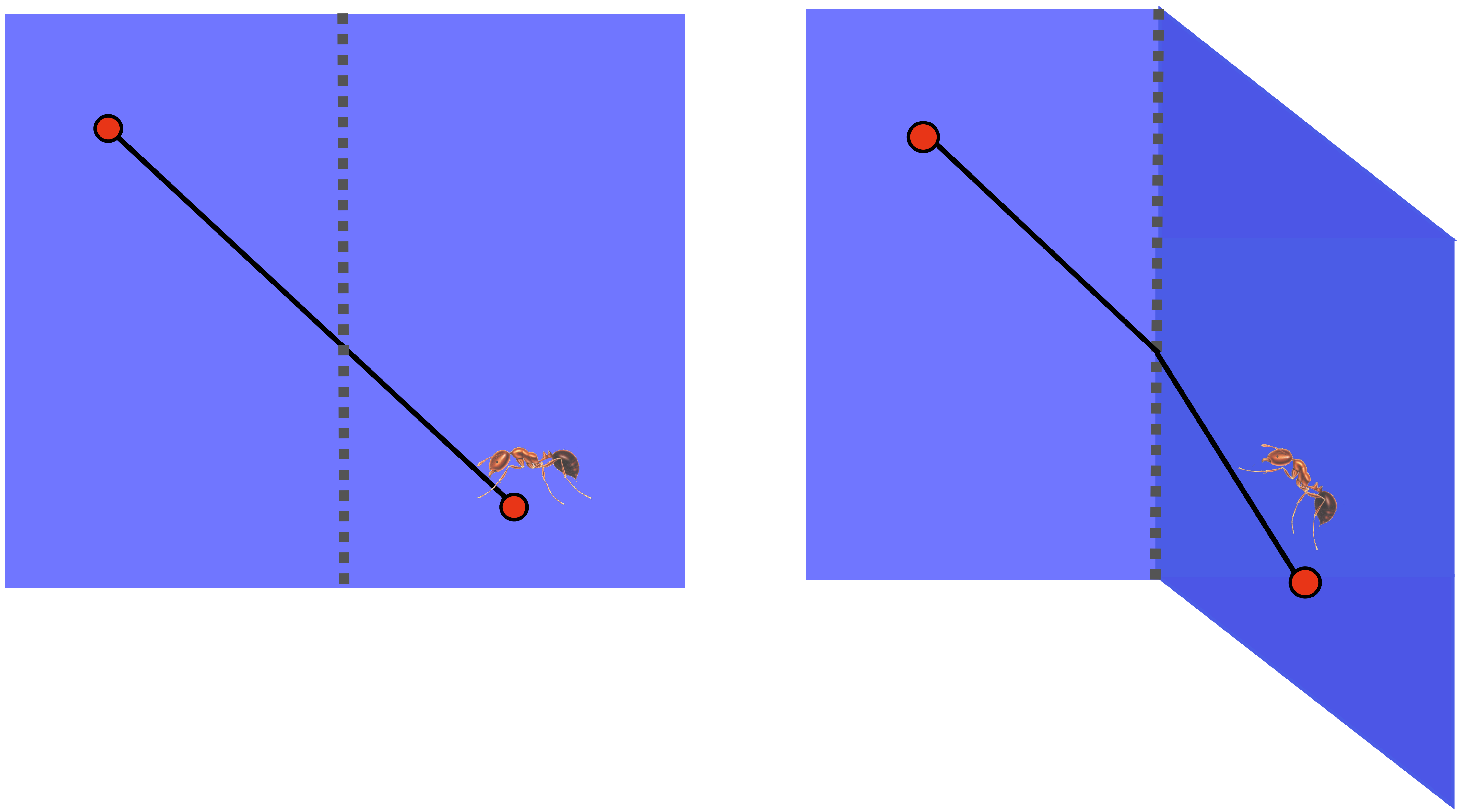
• **δ-Isometries**. Given a map $\phi : X \to Y$, we define its *distorsion* to be

$$\boxed{\operatorname{dis}(\phi) := \max_{x,x' \in X} |d_X(x, x') - d_Y(\phi(x), \phi(x'))| = \|d_X - d_Y \circ (\phi, \phi)\|_{L^\infty(X \times X)}.}$$

If $\phi : X \to Y$ is s.t. $\operatorname{dis}(\phi) \leq \delta$, and $\phi(X)$ is a δ-net for Y, then we say that ϕ is a δ-isometry.

Remark. *Note that if ϕ is a δ-isometry for $\delta = 0$, then ϕ is distance preserving. We will prove later on that this also forces ϕ to be a bijection. Then, 0-isometries are just isometries.*

Remark. *Recall bending transformations. We can now use the more appropriate term: isometries. We still need to specify what are the metric spaces we are talking about, though. So, in the example of the sheet of paper and the ant, the metric is the* intrinsic metric*.*



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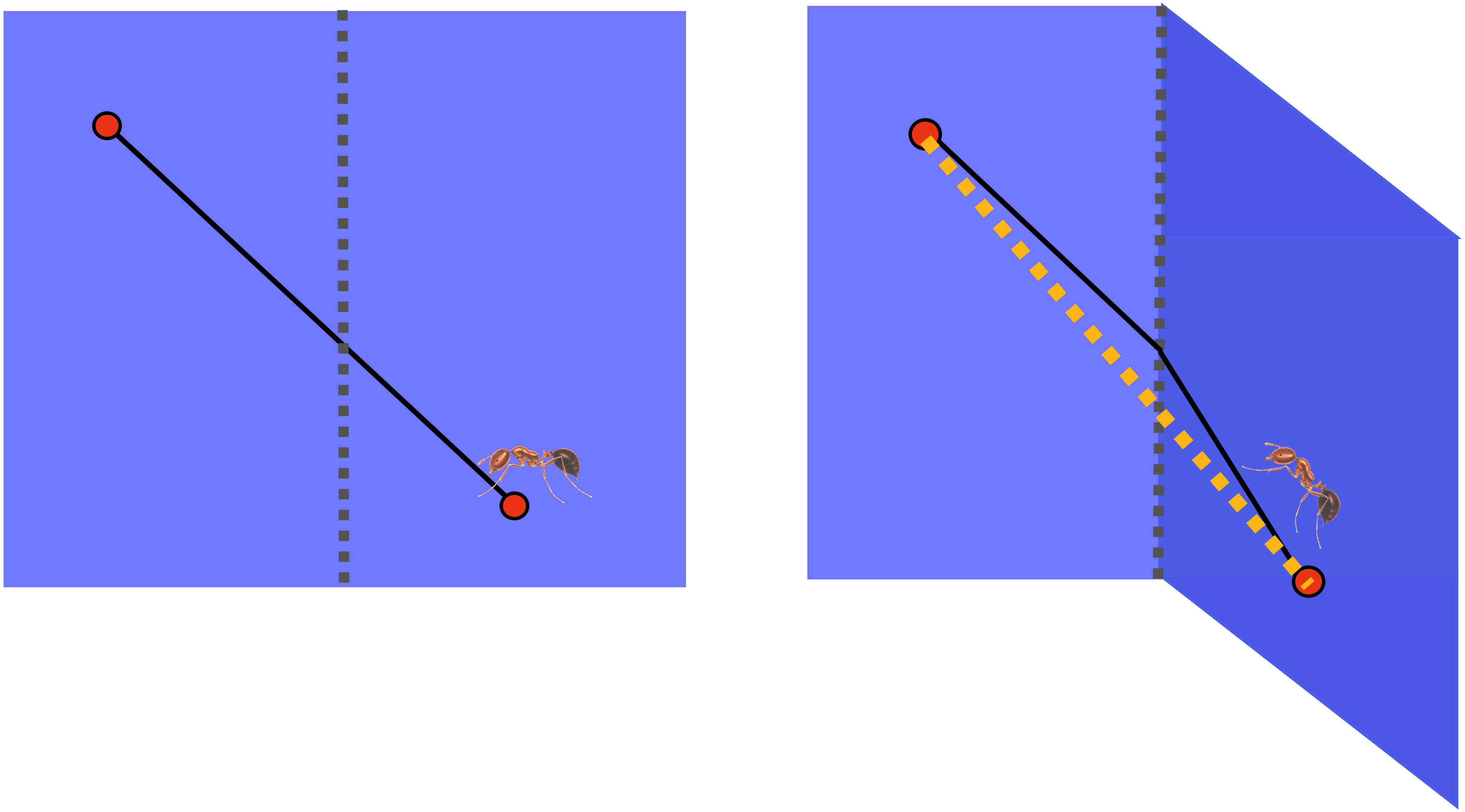

Remark. *Let* $\phi : X \to Y$ *and* $\psi : Y \to X$ *be given. Consider*

$$D(\phi, \psi) := \max(dis(\phi), dis(\psi)).$$

Question: if you have maps ϕ *and* ψ *s.t.* $D(\phi, \psi)$ *is small, do you think this will tell you something about how different* X *and* Y *are?*

• **Distance matrix**. Given a metric space (X, d) and a finite subset $\mathbb{X}$ of X, we form the matrix $\mathbf{D}(\mathbb{X})$ of all pairwise distances between points in $\mathbb{X}$. $\mathbf{D}(\mathbb{X})$ is called the distance matrix of $\mathbb{X}$.

• **Isometries in Euclidean space**. In $\mathbb{R}^d$, a map $\Phi : \mathbb{R}^d \to \mathbb{R}^d$ s.t. $\|x - x'\| = \|\Phi(x) - \Phi(x')\|$ for all $x, x' \in \mathbb{R}^d$ is called a *rigid isometry*. We denote the group of these transformations by $E(d)$. Note that translations, reflections, rotations and compositions of these are in $E(d)$.

• **Folklore Lemma**. Let $\mathbb{X}_n = \{x_1, \ldots, x_n\}$ and $\mathbb{Y}_n = \{y_1, \ldots, y_n\}$ be points in $\mathbb{R}^k$. If

$$\|x_i - x_j\| = \|y_i - y_j\|$$

for all i, j, then there exists a *rigid isometry* $T : \mathbb{R}^k \to \mathbb{R}^k$ s.t.

$$T(x_i) = y_i, \text{ for all } i$$

Remark. *Note that this means that we can detect whether two objects in* $\mathbb{R}^d$ *are the same up to rigid isometries by comparing their associated distance matrices. This lemma is <u>not trivial</u>!. From information about finitely many points you are able to prove the existence of* an ambient space isometry *that maps one set into the other.*

Summary

- When dealing with databases of objects, one needs a notion of dis-similarity between objects.
- This notion must take into account desired invariance (we saw two kinds, bendings and rigid isometries).
- Whenever comparing two objects, one needs to establish a pairing between points, one in object A, one in object B. We saw correspondences and measure couplings.
- We discussed two notions of dis-similarity suited for objects in say $\mathbb{R}^3$: the Hausdorff distance and the Wasserstein distance.
- Reading assignment for next class: start with **[M07]**, first 4 sections.
- We will start by looking into how to incorporate invariances into our notions of distance between objects.