Shape Matching: A Metric Geometry Approach Facundo Mémoli. CS 468, Stanford University, Fall 2008.

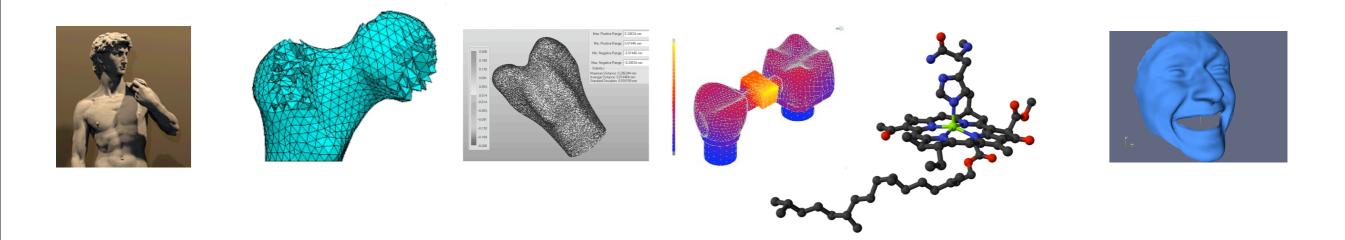


The Problem of Shape/Object Matching

- 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

- $\bullet\,$ assume you have database ${\cal D}$ 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} :

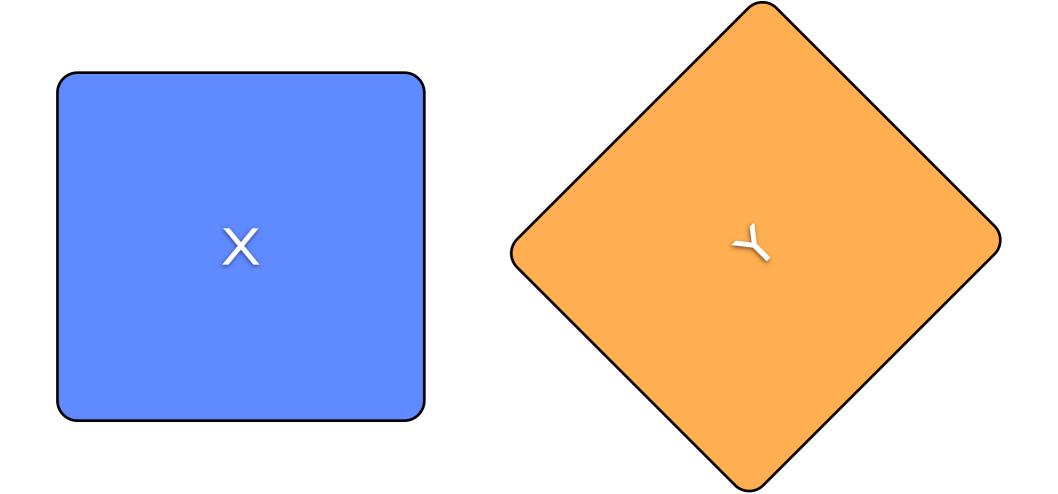
class(o) = class(z)

where $z \in \mathcal{D}$ 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*.

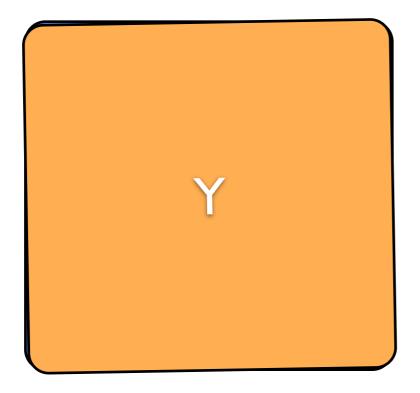
Another important point: invariances

Are these two objects the same?



Another important point: invariances

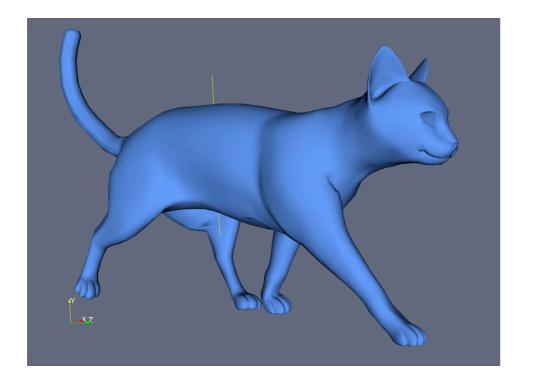
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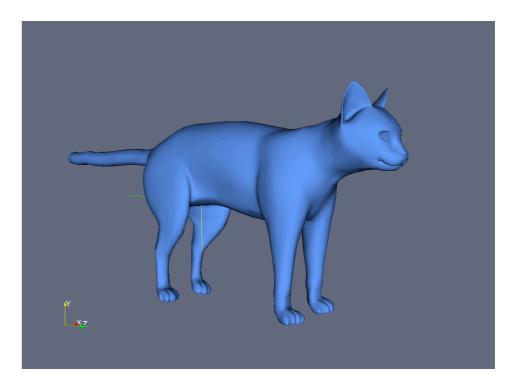


this is called invariance to *rigid transformations*

Another important points: invariances

what about these two?

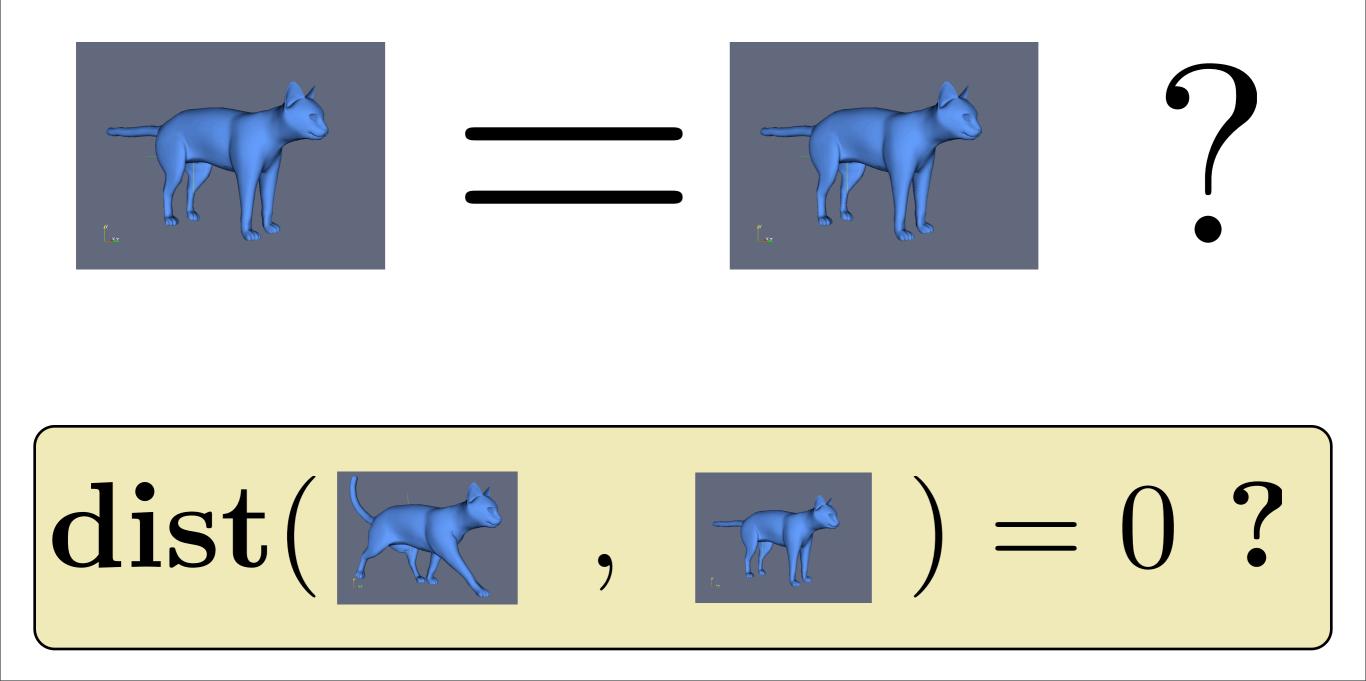




roughly speaking, this corresponds to invariance to *bending transformations*..

invariances...

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



What we proposed in the course:

- 1. Decide what *invariances* you wish to incorporate. It is OK if you don't have invariances (Hausdorff + Wasserstein)
- 2. Represent shapes as metric spaces (or mm-spaces):
 - Identify what metric is preserved by the notion of invariance you chose to consider.
 - Endow shapes with that metric
 - Choose weights that are meaningful for your application (if you don't have any reason to choose: then set them to be equal)
- 3. Define a *metric* on your class of objects.

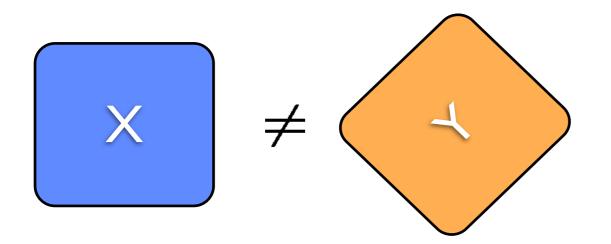
We studied the case of <u>no invariances</u> first.

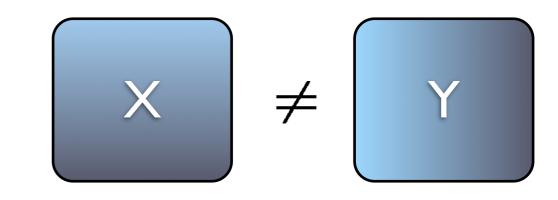
No invariances..

- You start out with a compact metric space (Z, d) (called *ambient space*, typically $Z = \mathbb{R}^k$).
- We saw two constructions:

$$(\mathcal{C}(Z), d_{\mathcal{H}}^Z)$$
 and $(\mathcal{C}_w(Z), d_{\mathcal{W}, p}^Z)$

where $\mathcal{C}(Z)$ stands for all compact subsets of Z and $\mathcal{C}_w(Z)$ for all weighted subsets of Z: that is, pairs (A, μ_A) where μ_A is a probability measure on Z s.t. supp $[\mu_A] = A$.



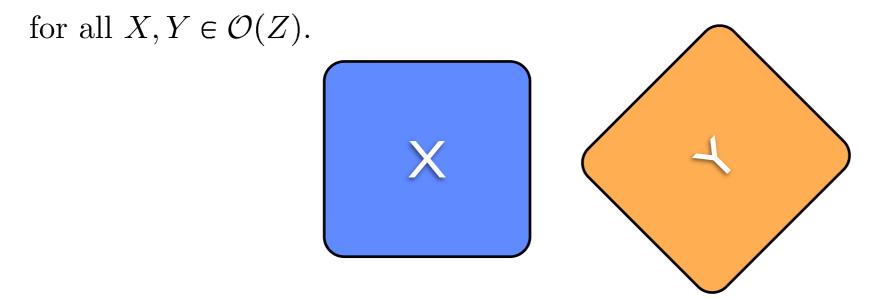


Ambient space isometries..(Extrinsic approach)

Fix a compact metric space (Z, d). Let I(Z) denote the isometry group of Z (when $Z = \mathbb{R}^k$, I(Z) = E(k), that is, all Euclidean isometries.)

- In this case, we considered either objects in $\mathcal{C}(Z)$ or in $\mathcal{C}_w(Z)$. Let $\mathcal{O}(Z)$ denote your choice.
- Let **dist** be the corresponding metric (Hausdorff or Wasserstein).
- Then, we constructed distances between objects in $\mathcal{O}(Z)$ that were <u>blind to isometries</u>:

$$\mathbf{dist}^{iso}(X,Y) := \inf_{T \in I(Z)} \mathbf{dist}(X,T(Y))$$



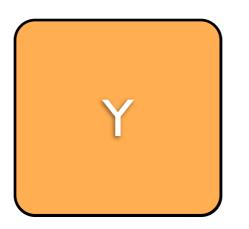
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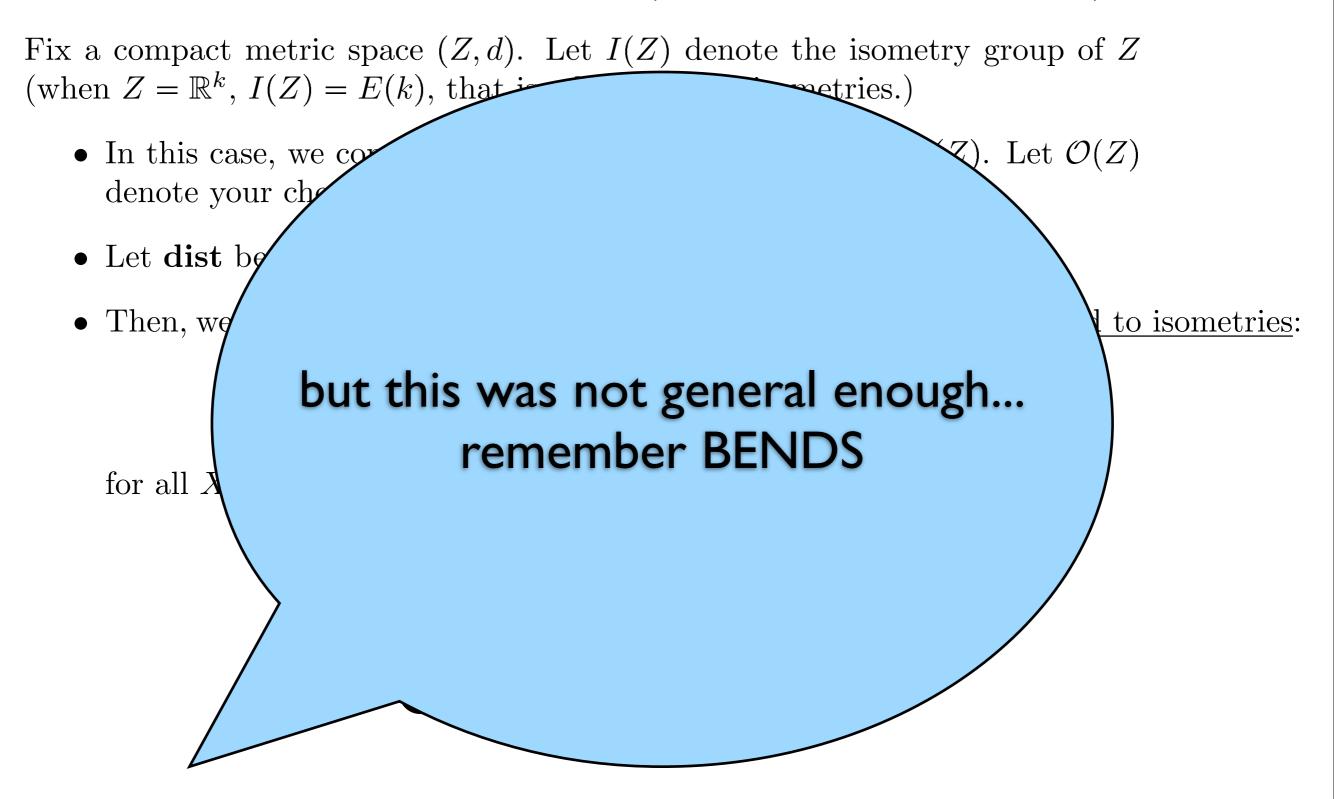
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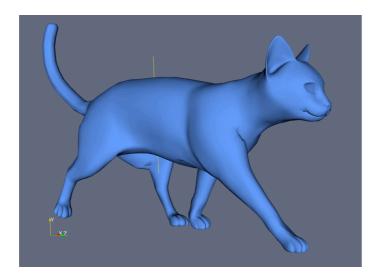
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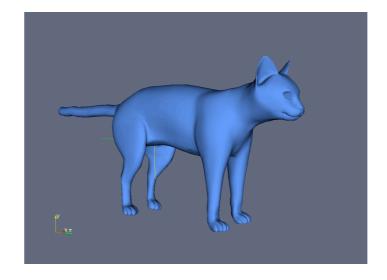
for all $X, Y \in \mathcal{O}(Z)$.

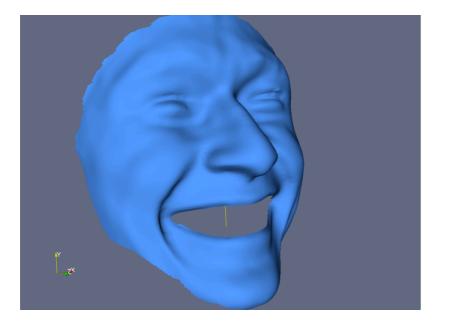


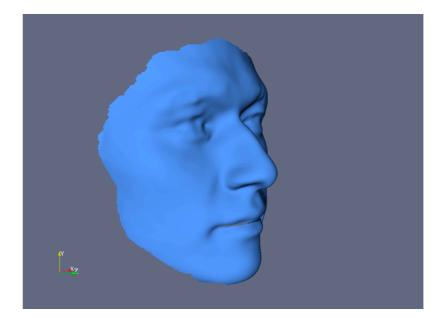
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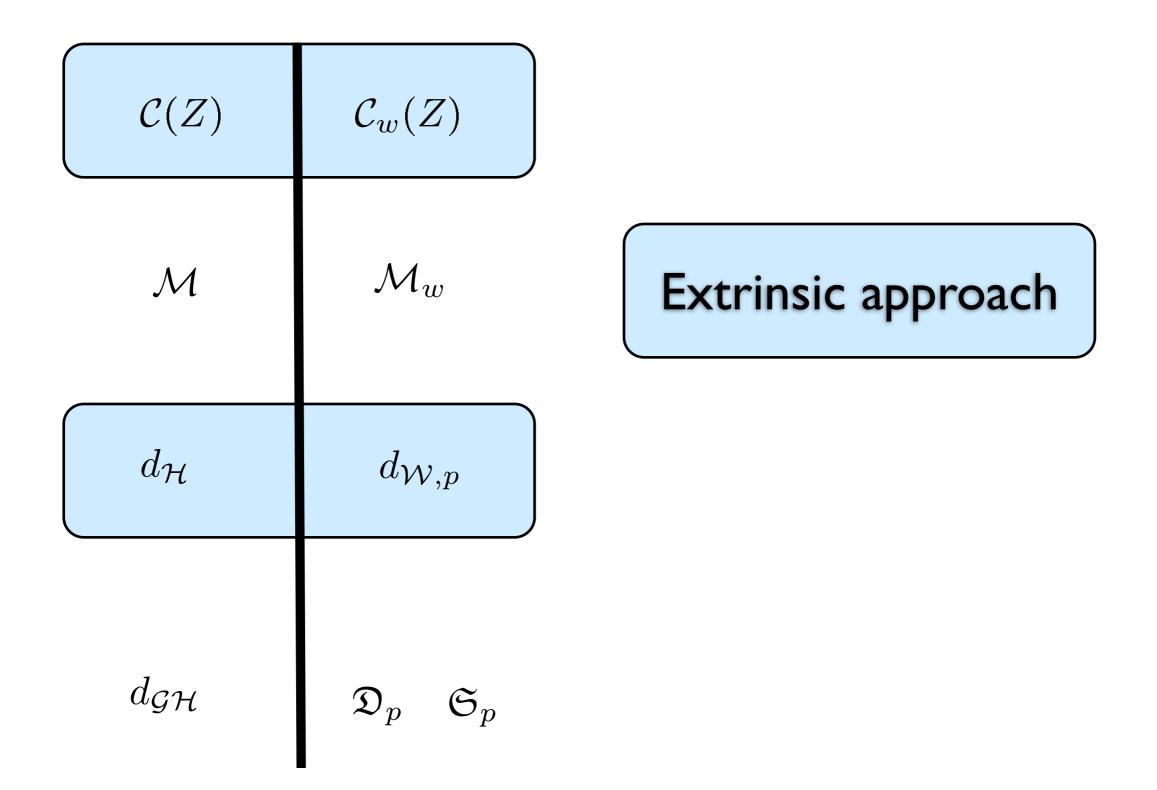






The intrinsic approach...

- Regard shapes as metric spaces in themselves: no reference to any ambient space.
- That is, objects/shapes now are metric spaces or mm-spaces (X, d_X) or (X, d_X, μ_X) .
- Let \mathcal{M} denote collection of all metric spaces and \mathcal{M}_w the collections of all mm-spaces.
- Endow \mathcal{M} and/or \mathcal{M}_w with a metric.
- We saw the following constructions:
 - On \mathcal{M} we put the Gromov-Hausdorff distance $d_{\mathcal{GH}}(,)$.
 - On \mathcal{M}_w we put two metrics, \mathfrak{S}_p and \mathfrak{D}_p . These metrics could be called Gromov-Wasserstein metrics.



$\mathcal{C}(Z)$	$\mathcal{C}_w(Z)$	
\mathcal{M}	\mathcal{M}_w	Extrinsic approach
$d_{\mathcal{H}}$	$d_{\mathcal{W},p}$	Intrinsic approach
$d_{\mathcal{GH}}$	\mathfrak{D}_p \mathfrak{S}_p	

What is the relationship between the Intrinsic and Extrinsic Approaches?

- Answer known for $Z = \mathbb{R}^k$, [M08-euclidean].
- In class we saw the case of $d_{\mathcal{GH}}$ vs. $d_{\mathcal{H}}^{iso}$: for all $X, Y \in \mathbb{R}^k$,

 $d_{\mathcal{GH}}((X, \|\cdot\|), (Y, \|\cdot\|)) \leq \inf_{T \in E(k)} d_{\mathcal{H}}(X, T(Y)) \leq C_k \left(d_{\mathcal{GH}}((X, \|\cdot\|), (Y, \|\cdot\|)) \right)^{1/2} M^{1/2}$

where $M = \max(\operatorname{diam}(X), \operatorname{diam}(Y))$.

• There is a similar claim valid for \mathfrak{S}_p vs. $d_{\mathcal{W},p}^{iso}$.

Main points

- Define notion of distance on shapes. Get sampling consistency + stability for free.
- GH distance leads to hard combinatorial optimization problems.
- Relaxations of these do not appear to be correct.
- Gromov-Wasserstein distances are better. Both \mathfrak{D}_p and \mathfrak{S}_p yield quadratic optimization probs. with linear constraints.
- Sturm's \mathfrak{S}_p requires large nbr. of constraints, then we argue for \mathfrak{D}_p .
- Many lower bounds for \mathfrak{D}_p are possible. These employ invariants previously used in the literature:
 - Shape Distributions
 - Eccentricities (Hamza-Krim)
 - Shape contexts

Main Technical concepts

- Metric spaces, mm-spaces, isometries, approximate isometries, probability measures.
- Correspondences, measure couplings, metric couplings.
- Hausdorff distance. Wasserstein distance. Mass transportation.
- Gromov-Hausdorff distance. Gromov-Wasserstein distances.
- Invariants of mm-spaces

correspondences and the Hausdorff distance

Definition [Correspondences]

For sets A and B, a subset $R \subset A \times B$ is a *correspondence* (between A and B) if 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. Note that in the case $n_A = n_B$, correspondences are larger than bijections.

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.

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

correspondences

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

Proposition

Let (X, d) be a compact metric space and $A, B \subset X$ be compact. Then

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

correspondences and measure couplings

Let (A, μ_A) and (B, μ_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 $((\mu_{a,b})) \in [0,1]^{n_A \times n_B}$)

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

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.

correspondences and measure couplings

Proposition $[(\mu \leftrightarrow R)]$

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

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

• König's Lemma. [gives conditions for $R \to \mu$]

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

 $\Downarrow (R \leftrightarrow \mu)$

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

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

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

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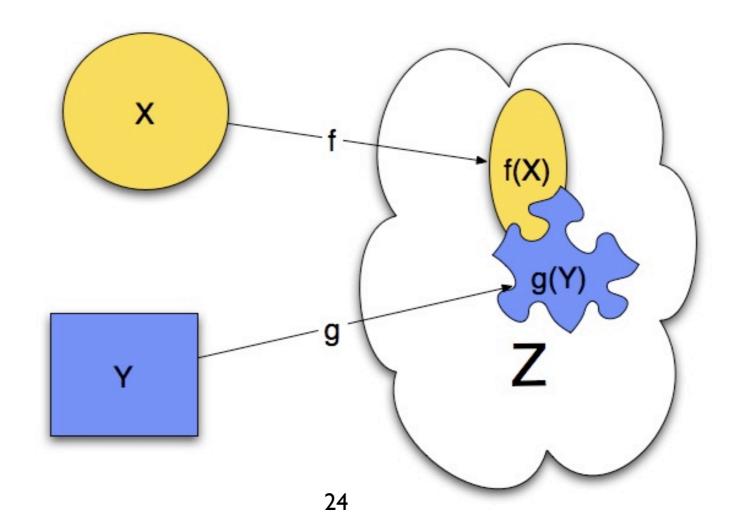
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$$d_{\mathcal{W},\mathbf{p}}(A,B) = \inf_{\mu \in \mathcal{M}(\mu_A,\mu_B)} \|d\|_{L^{\mathbf{p}}(A \times B,\mu)}$$

GH distance

GH: definition

$d_{\mathcal{GH}}(X,Y) = \inf_{Z,f,g} d_{\mathcal{H}}^Z(f(X),g(Y))$



correspondences and GH distance

The GH distance between (X, d_X) and (Y, d_Y) admits the following expression:

$$d_{\mathcal{GH}}^{(1)}(X,Y) = \inf_{d \in \mathcal{D}(d_X,d_Y)} \inf_{R \in \mathcal{R}(X,Y)} \|d\|_{L^{\infty}(R)}$$

where $\mathcal{D}(d_X, d_Y)$ is a metric on $X \sqcup Y$ that reduces to d_X and d_Y on $X \times X$ and $Y \times Y$, respectively.

$$\begin{array}{ccc} X & Y \\ X & \begin{pmatrix} d_X & \mathbf{D} \\ \mathbf{D}^T & d_Y \end{pmatrix} = d \end{array}$$

In other words: you need to glue X and Y in an optimal way. Note that **D** consists of $n_X \times n_Y$ positive reals that must satisfy $\sim n_X \cdot C_2^{n_Y} + n_Y \cdot C_2^{n_X}$ linear constraints.

Another expression for the GH distance

For compact spaces (X, d_X) and (Y, d_Y) let

$$d_{\mathcal{GH}}^{(2)}(X,Y) = \frac{1}{2} \inf_{R} \max_{(x,y),(x',y')\in R} |d_X(x,x') - d_Y(y,y')|$$

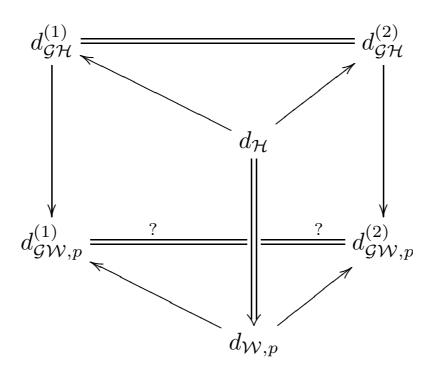
We write, compactly,

$$d_{\mathcal{GH}}^{(2)}(X,Y) = \frac{1}{2} \inf_{R} \|d_X - d_Y\|_{L^{\infty}(R \times R)}$$

Equivalence thm:

Theorem [Kalton-Ostrovskii] For all X, Y compact,

Relaxing the notion of correspondence from GH to GW



Shapes as mm-spaces, [M07]

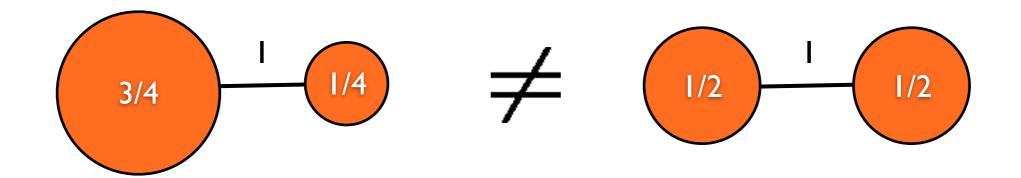
Remember:

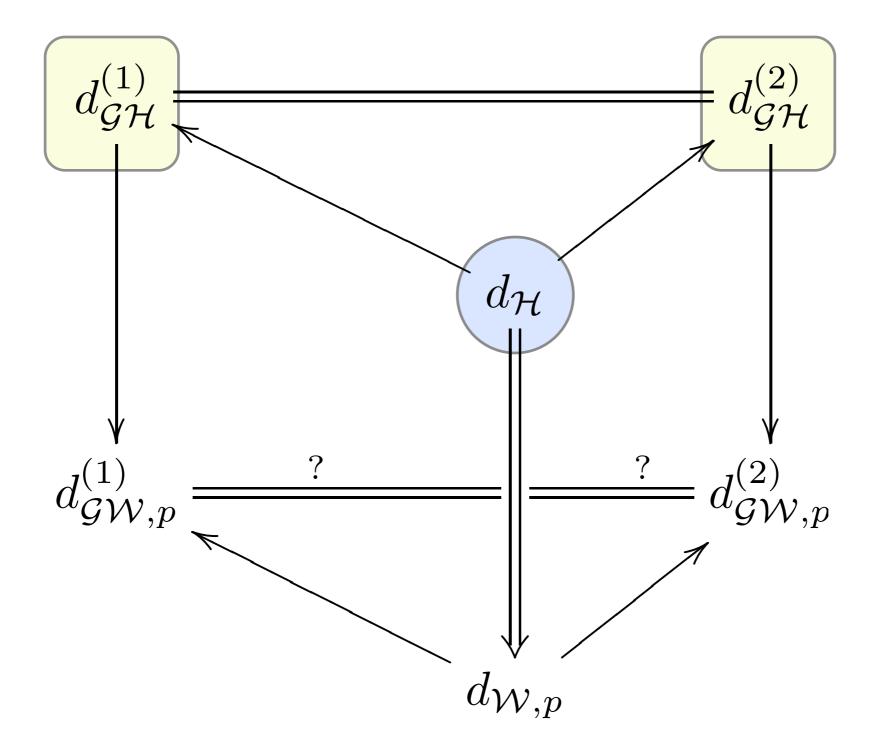
 (X, d_X, μ_X)

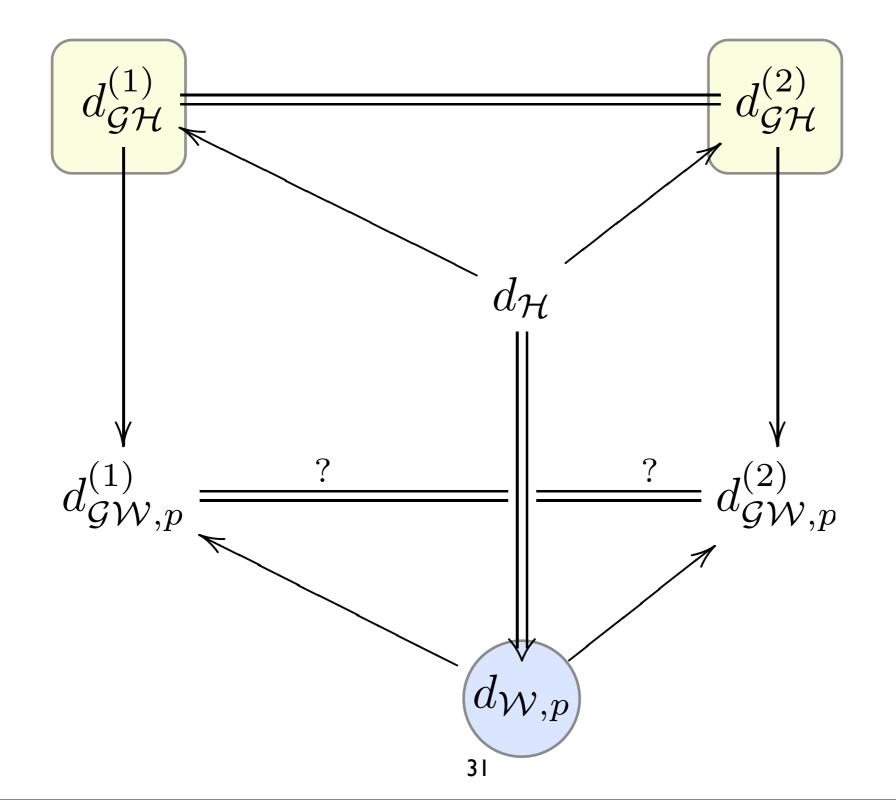
- 1. Specify representation of shapes.
- 2. Identify invariances that you want to mod out.
- 3. Describe notion of isomorphism between shapes (this is going to be the zero of your metric)
- 4. Come up with a *metric* between shapes (in the representation of 1.)
- Now we are talking of triples (X, d_X, μ_X) where X is a set, d_X a metric on X and μ_X a probability measure on X.
- These objects are called *measure metric spaces*, or mm-spaces for short.
- two mm-spaces X and Y are deemed equal or isomorphic whenever there exists an isometry $\Phi: X \to Y$ s.t. $\mu_Y(B) = \mu_X(\Phi^{-1}(B))$ for all (measurable) sets $B \subset Y$.

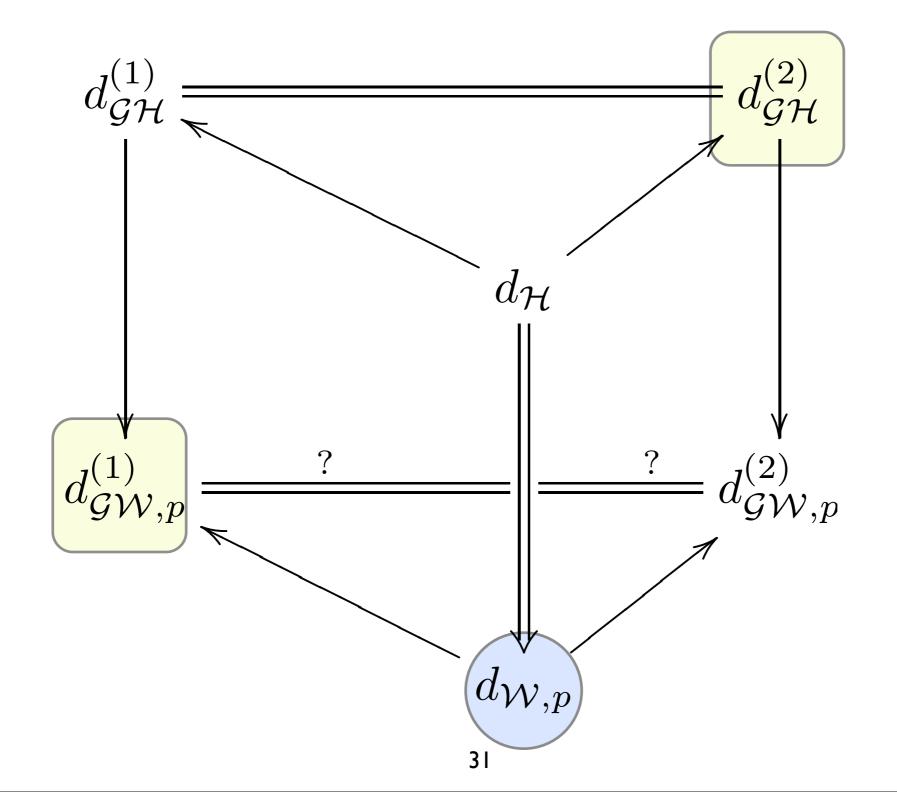
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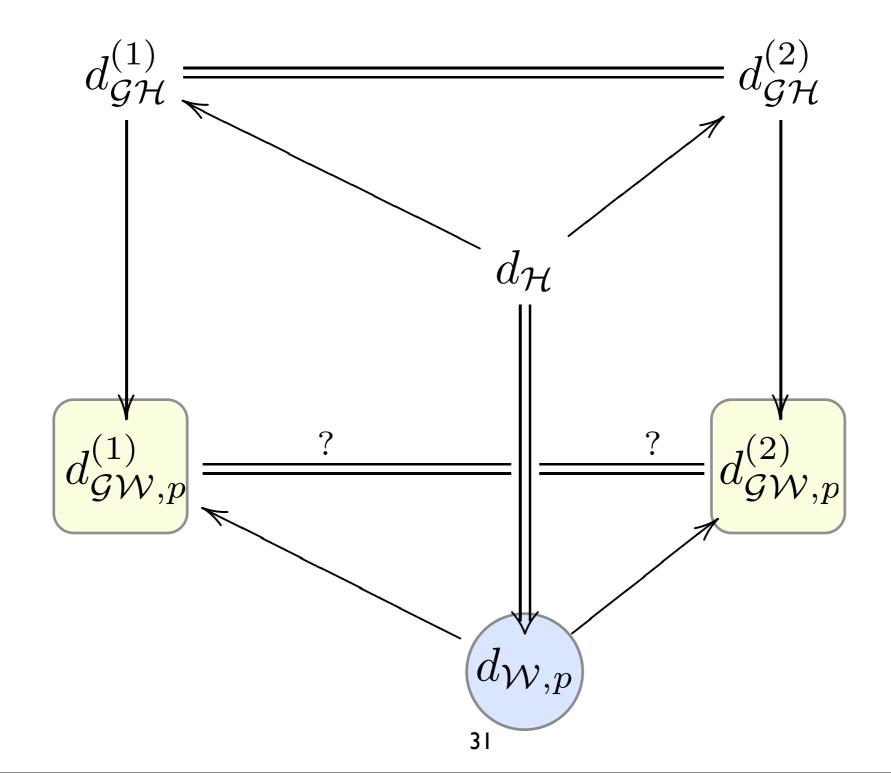
Now, one works with **mm-spaces**: triples (X, d, ν) where (X, d) is a compact metric space and ν is a Borel probability measure. Two mm-spaces are *iso*morphic iff there exists isometry $\Phi : X \to Y$ s.t. $\mu_X(\Phi^{-1}(B)) = \mu_Y(B)$ for all measurable $B \subset Y$.

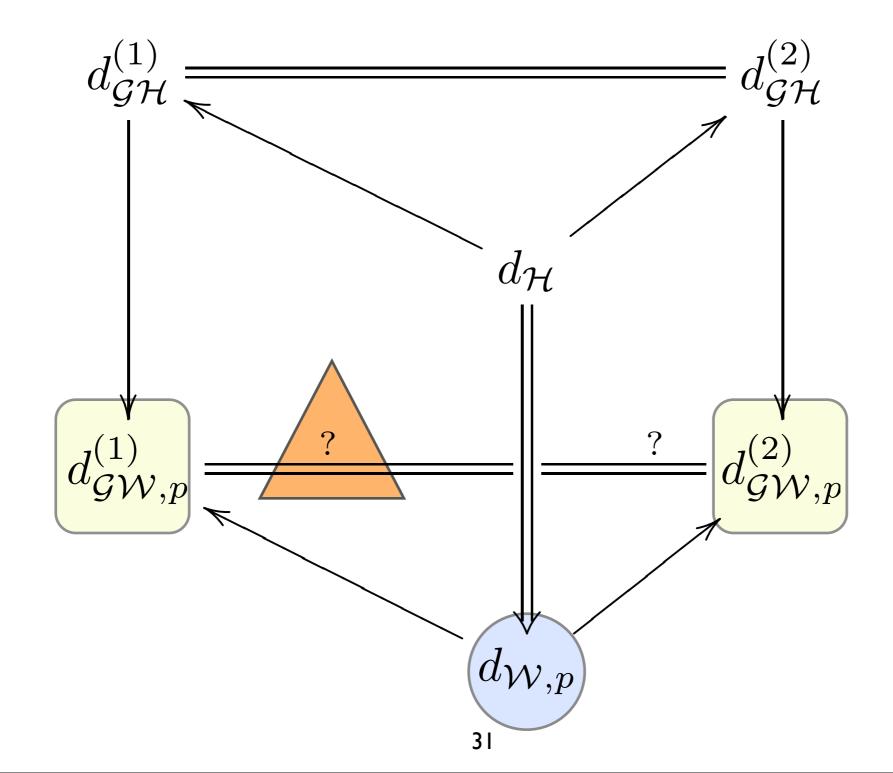


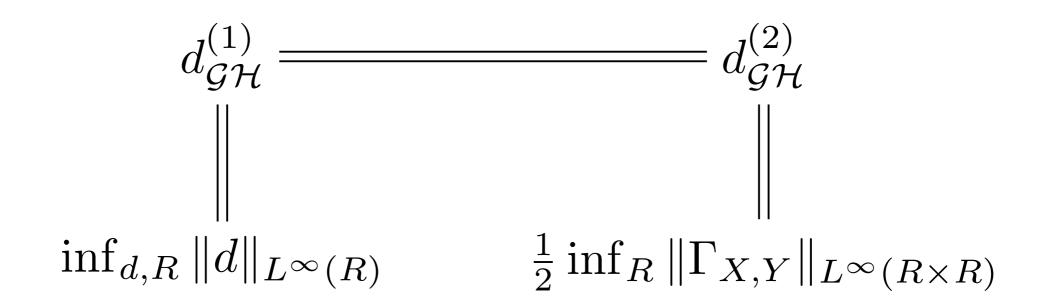


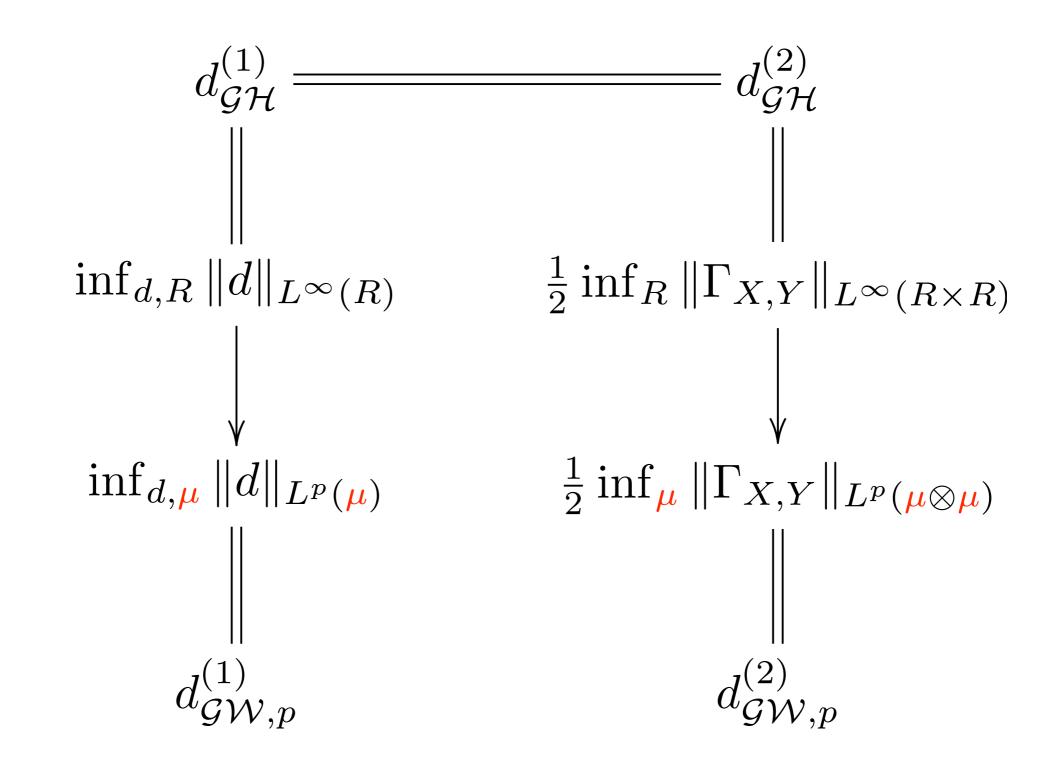


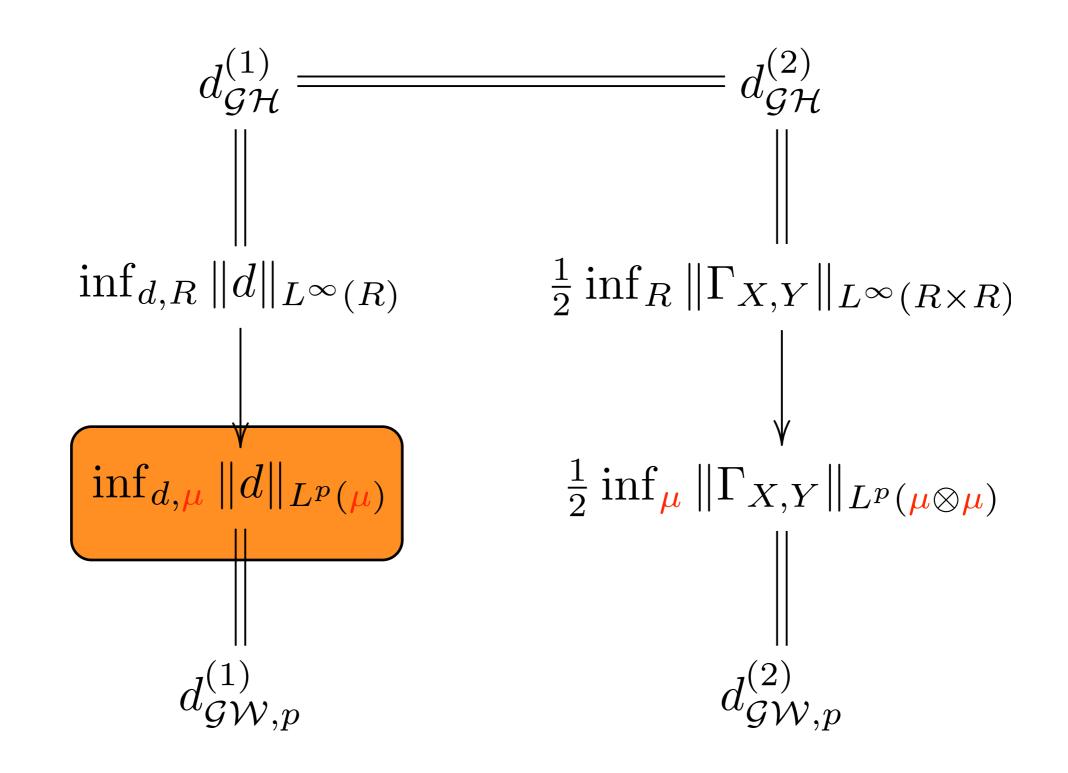


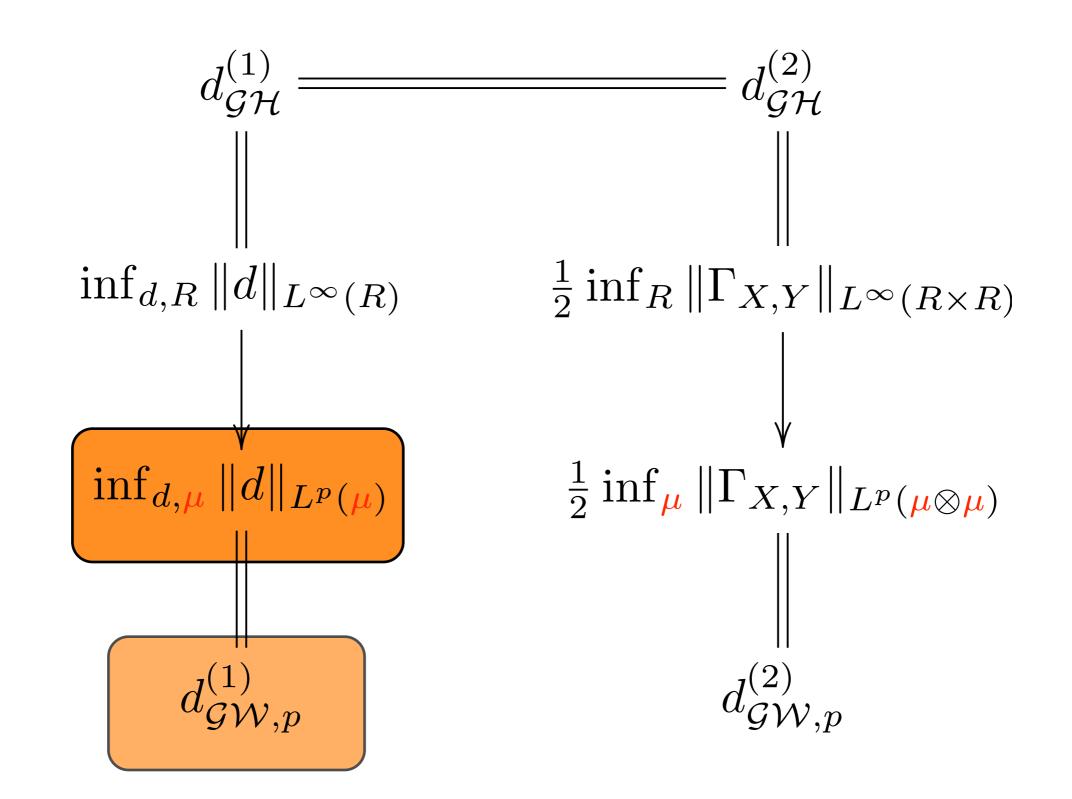


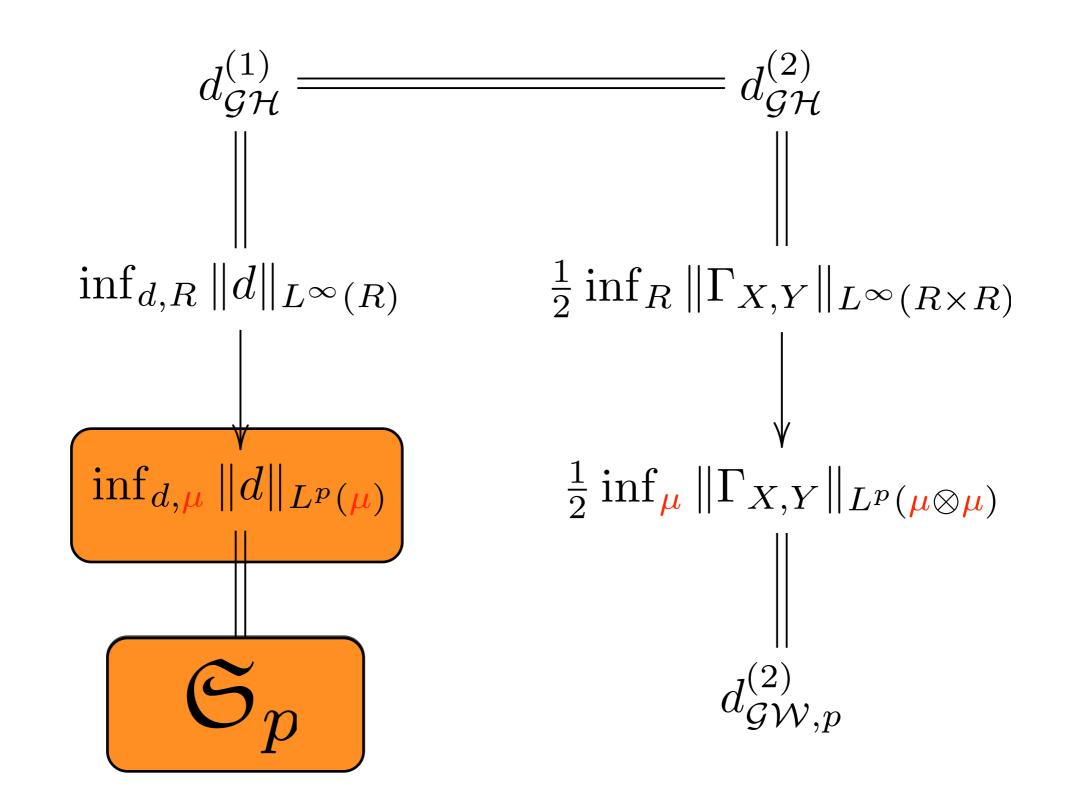


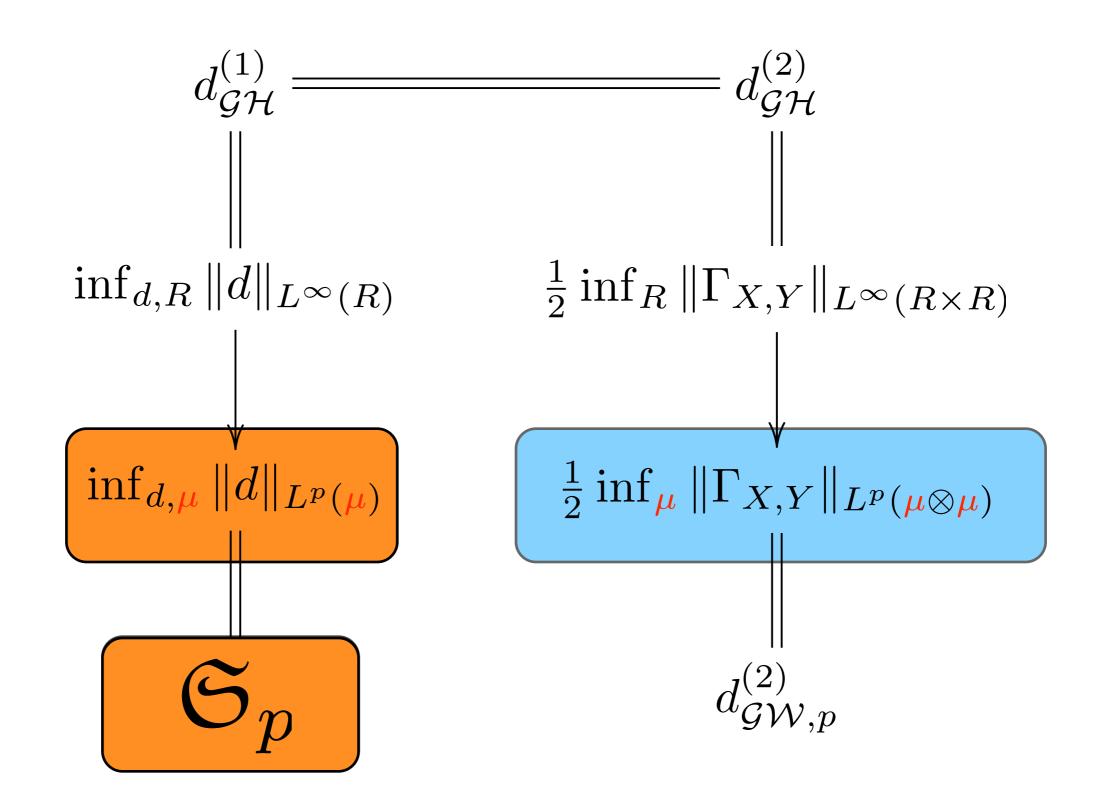


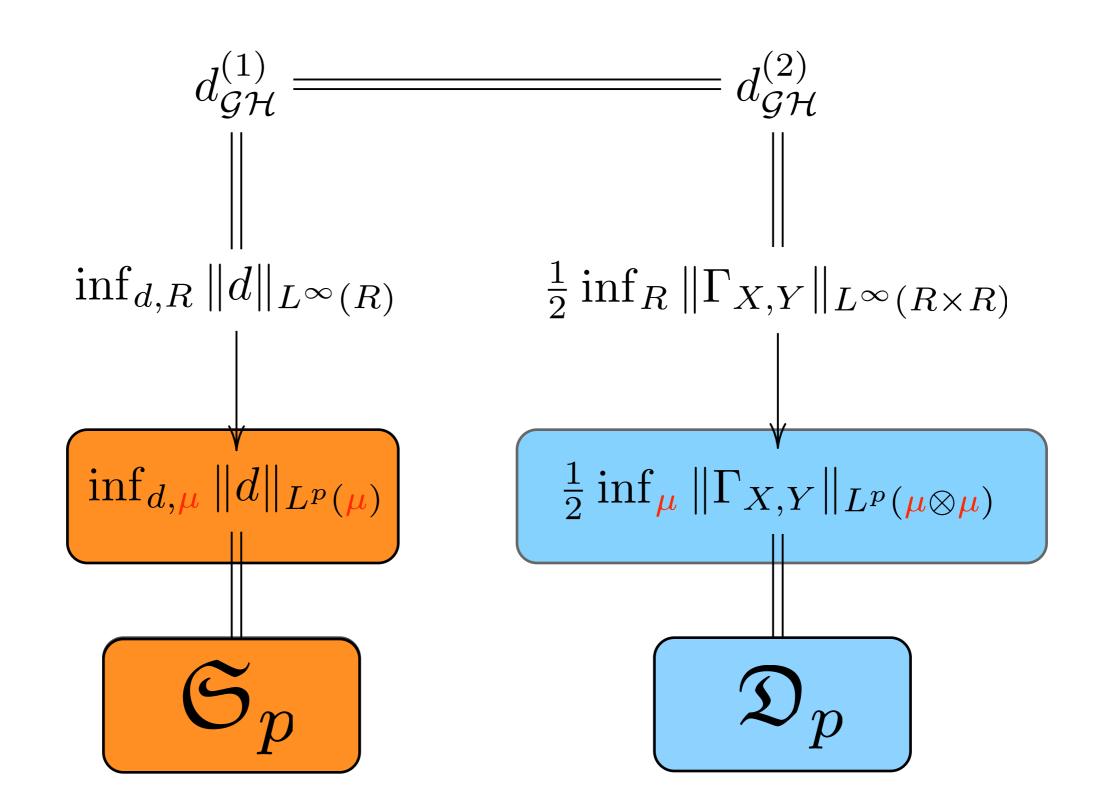












Can \mathfrak{S}_p be equal to \mathfrak{D}_p ?

• Using the same proof as in the Kalton-Ostrovskii Thm., one can prove that

$$\mathfrak{S}_{\infty}=\mathfrak{D}_{\infty}.$$

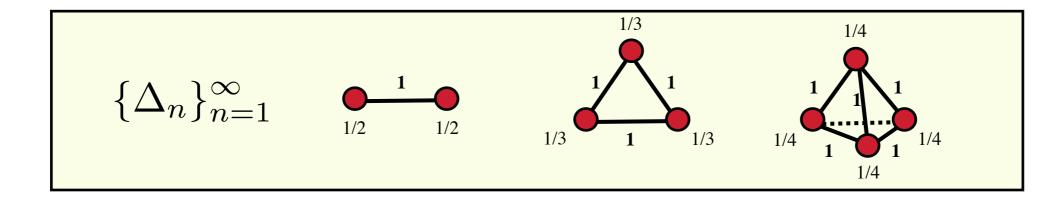
• Also, it is easy to see that for all $p \ge 1$

$$\mathfrak{S}_p \geq \mathfrak{D}_p.$$

• But the equality does not hold in general. One counterexample is as follows: take $X = (\Delta_{n-1}, ((d_{ij} = 1)), (\nu_i = 1/n))$ and $Y = (\{q\}, ((0)), (1))$. Then, for $p \in [1, \infty)$

$$\mathfrak{S}_1(X,Y) = \frac{1}{2} > \frac{1}{2} \left(\frac{n-1}{n}\right)^{1/p} = \mathfrak{D}_1(X,Y)$$

- Furthermore, these two (tentative) distances are **not Lipschitz equiv**alent!! This forces us to analyze them separately. The delicate step is proving that dist(X, Y) = 0 implies $X \simeq Y$.
- K. T. Sturm has analyzed \mathfrak{S}_p . Analysis of \mathfrak{D}_p is in [M07].



Properties of \mathfrak{D}_p

Theorem 1 ([M07]). 1. Let X, Y and Z mm-spaces then

 $\mathfrak{D}_p(X,Y) \leq \mathfrak{D}_p(X,Z) + \mathfrak{D}_p(Y,Z).$

2. If $\mathfrak{D}_p(X, Y) = 0$ then X and Y are isomorphic.

3. Let $X_n = \{x_1, \ldots, x_n\} \subset X$ be a subset of the mm-space (X, d, ν) . Endow X_n with the metric d and a prob. measure ν_n , then

 $\mathfrak{D}_p(X,\mathbb{X}_n) \leqslant d_{\mathcal{W},p}(\nu,\nu_n).$

4. $p \ge q \ge 1$, then $\mathfrak{D}_p \ge \mathfrak{D}_q$.

5. $\mathfrak{D}_{\infty} \geq d_{\mathcal{GH}}$.

The parameter p is not superfluous

For $p \in [1, \infty]$ let $\operatorname{diam}_p(X) = ||d_X||_{L^p(\mu_X \otimes \mu_X)}$.

The simplest lower bound for \mathfrak{D}_p one has is based on the triangle inequality plus the observation that

$$\mathfrak{D}_p((X, d_X, \mu_X), (\{q\}, 0, 1)) = \operatorname{diam}_p(X)$$

Then,

$$\mathfrak{D}_p(X,Y) \ge \frac{1}{2} |\operatorname{diam}_p(X) - \operatorname{diam}_p(Y)|$$

For example, when $X = S^n$ (spheres with uniform measure and usual intrinsic metric):

- $p = \infty$ gives $\operatorname{diam}_{\infty}(S^n) = \pi$ for all $n \in \mathbb{N}$
- p = 1 gives $\operatorname{diam}_1(S^n) = \pi/2$ for all $n \in \mathbb{N}$

•
$$p = 2$$
 gives $\operatorname{diam}_2(S^1) = \pi/\sqrt{3}$ and $\operatorname{diam}_2(S^2) = \sqrt{\pi^2/2 - 2}$

Lower bounds for \mathfrak{D}_p in terms of invariants

. Recall the invariants we defined before. Fix $X \in \mathcal{G}_w$ and $p \ge 1$.

• distribution of distances: $F_X : [0, \infty) \rightarrow [0, 1]$,

$$t \mapsto (\mu_X \otimes \mu_X)(\{(x, x') | d_X(x, x') \leq t\}).$$

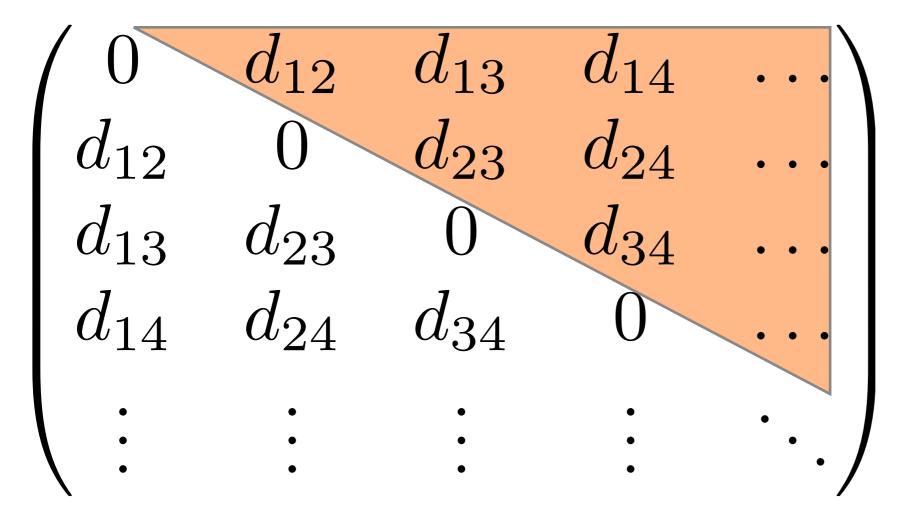
• local distribution of distances: $C_X : X \times [0, \infty) \rightarrow [0, 1],$

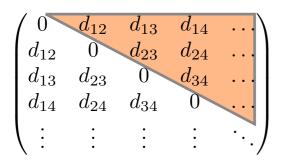
$$t \mapsto \mu_X(\{x' \mid d_X(x, x') \leqslant t\}).$$

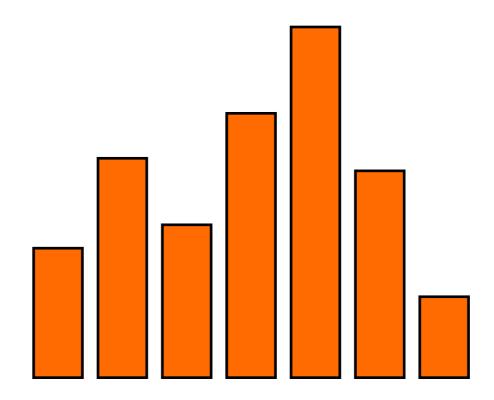
• eccentricities: $s_{X,p}: X \to \mathbb{R}^+$,

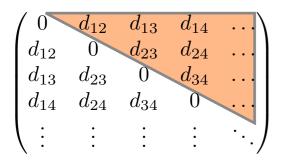
$$x \mapsto \|d_X(x, \cdot)\|_{L^p(\mu_X)}.$$

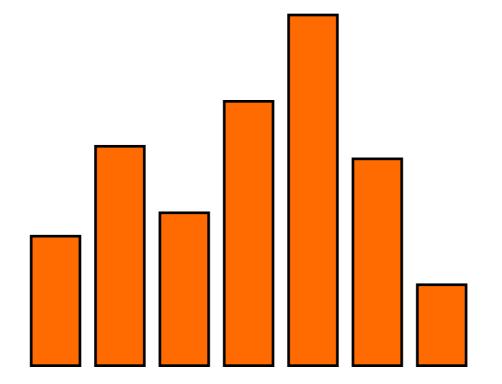
- There are explicit lower bounds for \mathfrak{D}_p in terms of these invariants, [M07].
- These lower bounds are important in practice: yield LOPs, easy optimization problems.
 Solution can be used as initial condition for solving \$\mathcal{D}_p\$.

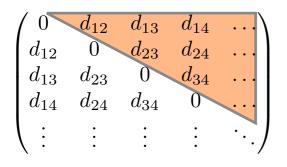


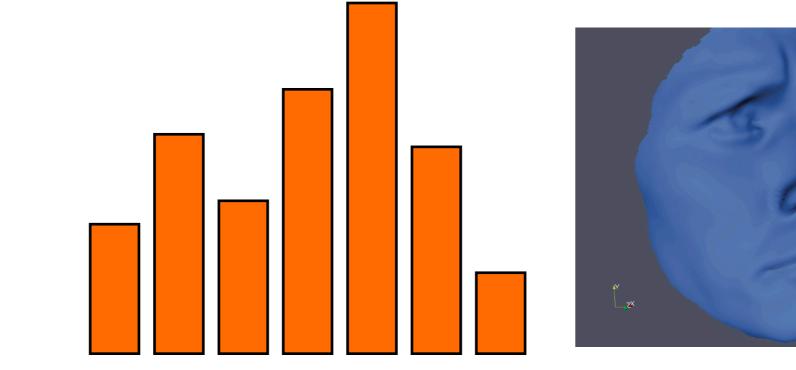


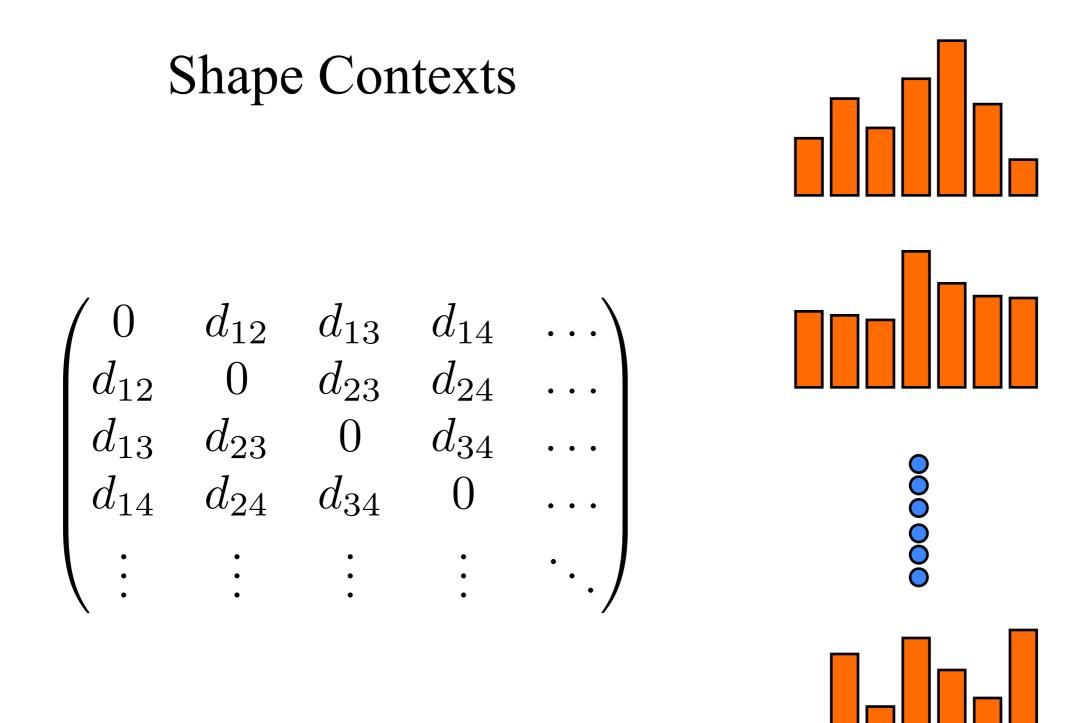


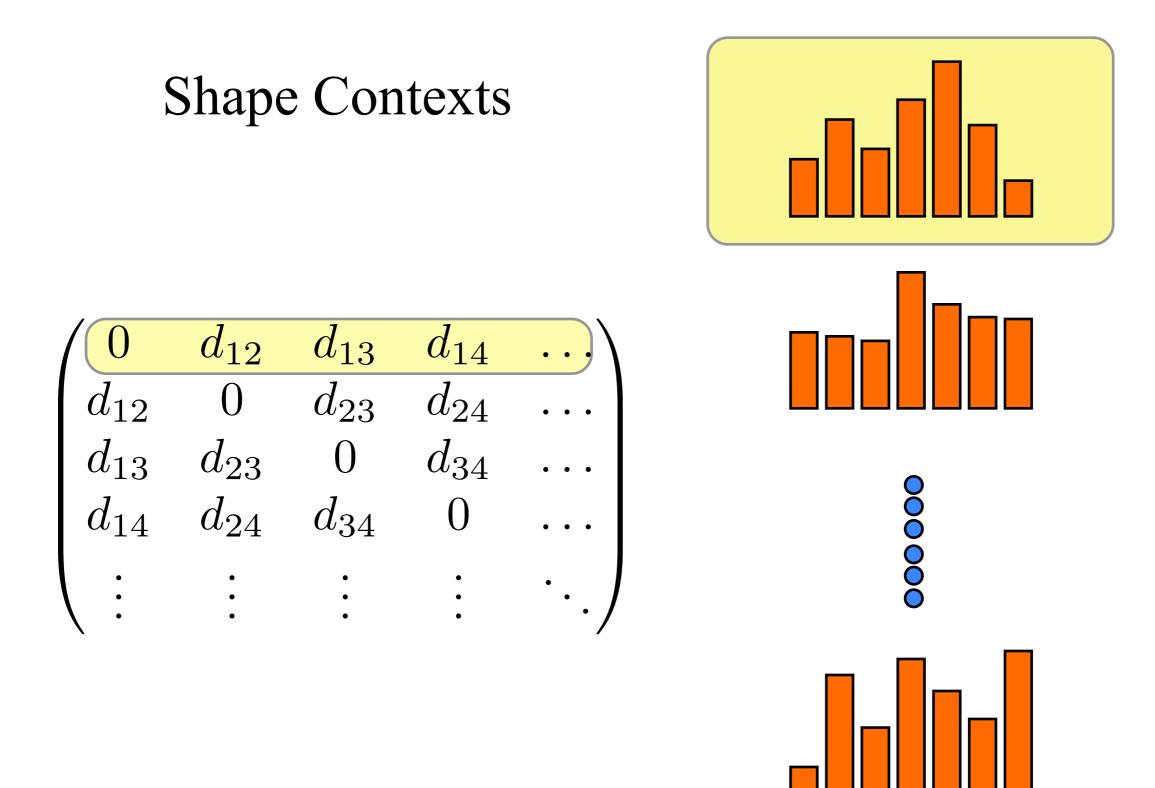


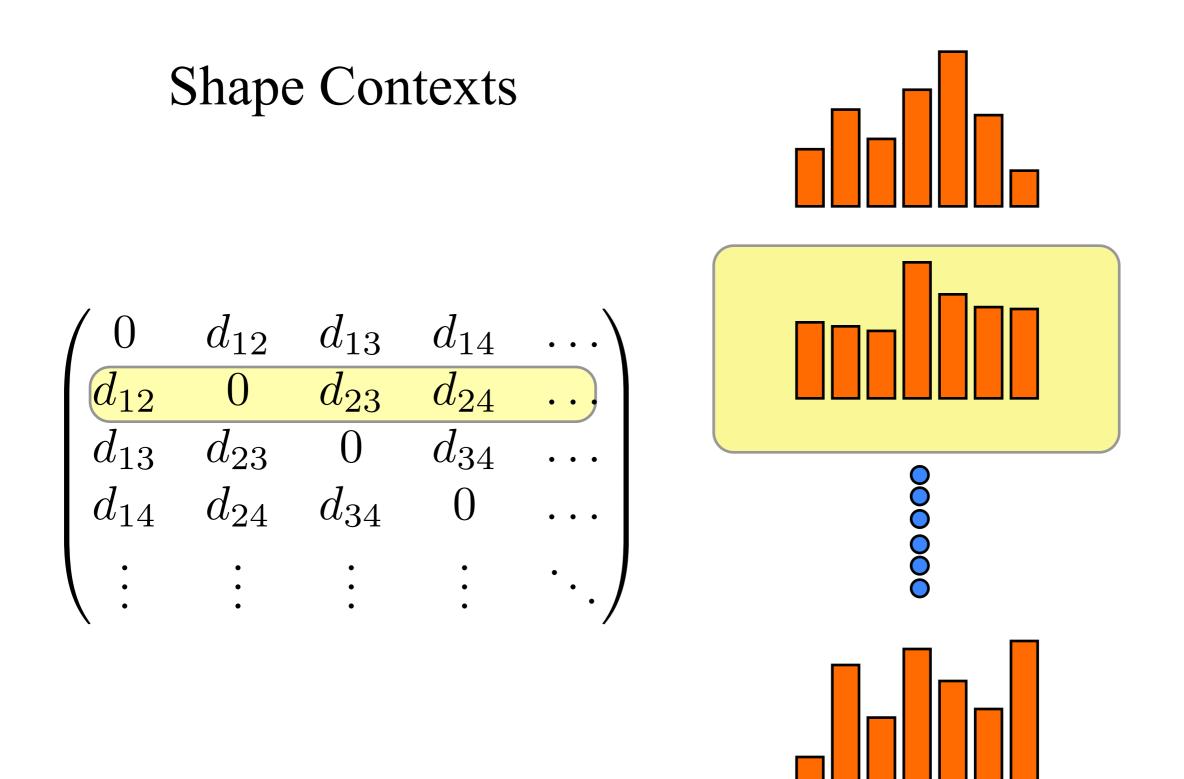












Hamza-Krim

 $\frac{\sum_j d_{1,j}}{N}$

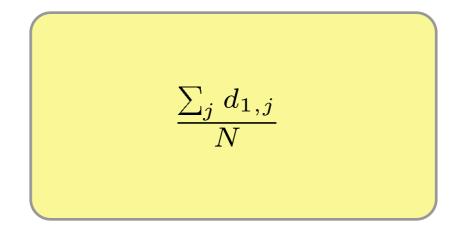
 $\begin{pmatrix} 0 & d_{12} & d_{13} & d_{14} & \dots \\ d_{12} & 0 & d_{23} & d_{24} & \dots \\ d_{13} & d_{23} & 0 & d_{34} & \dots \\ d_{14} & d_{24} & d_{34} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$

 $\frac{\sum_j d_{2,j}}{N}$ 000000



 $\frac{\sum_j d_{N,j}}{N}$

Hamza-Krim



$\left(\begin{array}{c} 0 \end{array} \right)$	d_{12}	d_{13}	d_{14}	
d_{12}	0	d_{23}	d_{24}	•••
d_{13}	d_{23}	0	d_{34}	• • •
d_{14}	d_{24}	d_{34}	0	• • •
	•	•	•	·.)

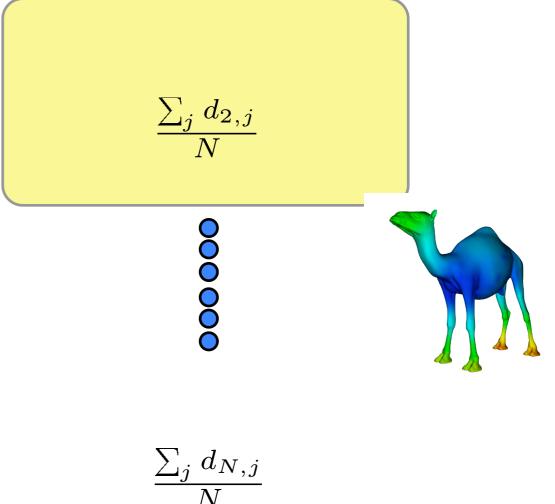
 $\frac{\sum_j d_{2,j}}{N}$ 000000

 $\frac{\sum_j d_{N,j}}{N}$

Hamza-Krim

 $\frac{\sum_j d_{1,j}}{N}$

 $\begin{pmatrix} 0 & d_{12} & d_{13} & d_{14} & \dots \\ d_{12} & 0 & d_{23} & d_{24} & \dots \\ d_{13} & d_{23} & 0 & d_{34} & \dots \\ d_{14} & d_{24} & d_{34} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$



The discrete case.

The option proposed and analyzed by K.L Sturm [St06], reads

$$\mathfrak{S}_p(X,Y) = \inf_{\boldsymbol{d}\in\mathcal{D}(d_X,d_Y)} \inf_{\boldsymbol{\mu}\in\mathcal{M}(\mu_X,\mu_Y)} \left(\sum_{x,y} \boldsymbol{d}^p(x,y)\boldsymbol{\mu}_{x,y}\right)^{1/p}$$

The second option reads [M07]

$$\mathfrak{D}_{p}(X,Y) = \inf_{\mu \in \mathcal{M}(\mu_{X},\mu_{Y})} \left(\sum_{x,y} \sum_{x',y'} |d_{X}(x,x') - d_{Y}(y,y')|^{p} \mu_{x,y} \mu_{x',y'} \right)^{1/p}$$

The **first** option,

$$\mathfrak{S}_p = \inf_{\boldsymbol{d}\in\mathcal{D}(d_X,d_Y)} \inf_{\boldsymbol{\mu}\in\mathcal{M}(\mu_X,\mu_Y)} \left(\sum_{x,y} \boldsymbol{d}^p(x,y)\boldsymbol{\mu}_{x,y}\right)^{1/p}$$

requires $2(\mathbf{n}_{\mathbf{X}} \times \mathbf{n}_{\mathbf{Y}})$ variables and $\mathbf{n}_{\mathbf{X}} + \mathbf{n}_{\mathbf{Y}}$ plus $\sim \mathbf{n}_{\mathbf{Y}} \cdot \mathbf{C}_{2}^{\mathbf{n}_{\mathbf{X}}} + \mathbf{n}_{\mathbf{X}} \cdot \mathbf{C}_{2}^{\mathbf{n}_{\mathbf{Y}}}$ linear constraints. When p = 1 it yields a *bilinear* optimization problem.

Our second option,

$$\mathfrak{D}_{p}(X,Y) = \inf_{\mu \in \mathcal{M}(\mu_{X},\mu_{Y})} \left(\sum_{x,y} \sum_{x',y'} |d_{X}(x,x') - d_{Y}(y,y')|^{p} \mu_{x,y} \mu_{x',y'} \right)^{1/p}$$

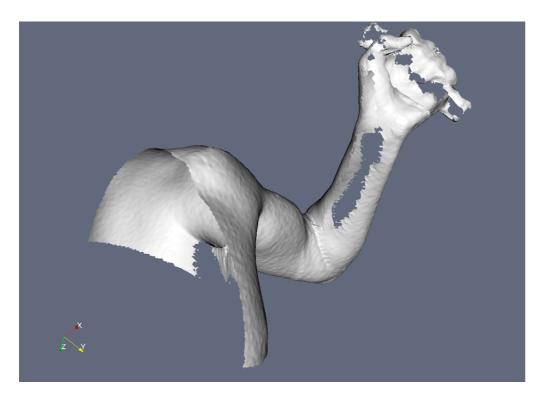
requires $\mathbf{n}_{\mathbf{X}} \times \mathbf{n}_{\mathbf{Y}}$ variables and $\mathbf{n}_{\mathbf{X}} + \mathbf{n}_{\mathbf{Y}}$ linear constraints. It is a *quadratic* (generally non-convex :-() optimization problem (with linear and bound constraints) for all p.

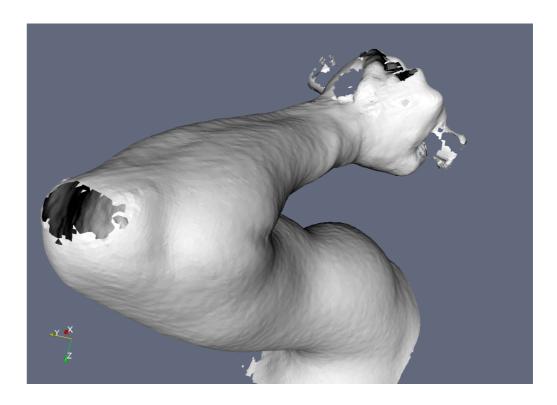
Future

- Study families of shapes.
- Statistic of families of shapes.
- Partial shape matching.
- Connections with Persistent topology invariants (Frosini+others... Yi will describe Frosini's work)
- Comparison/matching of animated geometries (Peter will talk about this)

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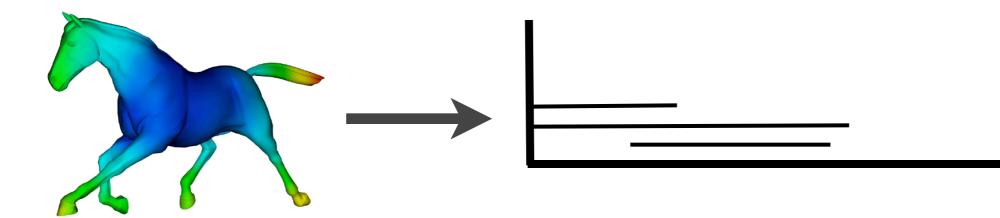
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and more

- Explain/relate more methods using these ideas: what about eigenvalue based methods?
 - Shape signatures [Reuter-et-al]: associate to each shape the sorted list of eigenvalues of the Laplacian on the shape.
 - Leordaneau... from matching of pairs of points to matching of points.
- The GH distance and related Metric Geometry ideas are very powerful and can probably help uniformizing the treatment of many algorithmic procedure out there.

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http://math.stanford.edu/~memoli