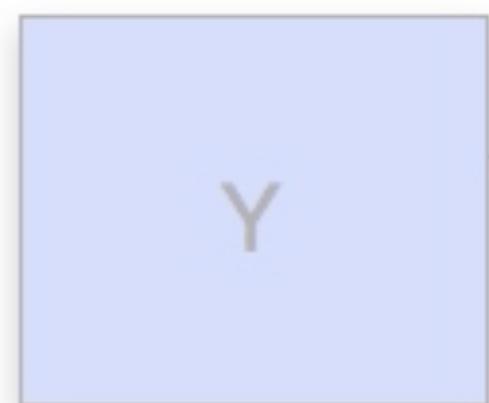


Shape Matching using Gromov-Hausdorff distances



Facundo Mémoli

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Background concepts

- **Metric Space.** A metric space is a pair (X, d) where X is a set and $d : X \times X \rightarrow \mathbb{R}^+$ 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 $x = y$.
- **Folklore Lemma.** Let $\mathbb{X}_n = \{x_1, \dots, x_n\}$ and $\mathbb{Y}_n = \{y_1, \dots, y_n\}$ 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* $T : \mathbb{R}^k \rightarrow \mathbb{R}^k$ s.t.

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

Let $\mathbf{D}(\mathbb{X}_n)$ and $\mathbf{D}(\mathbb{Y}_m)$ be the Euclidean interpoint distance matrices of \mathbb{X}_n and \mathbb{Y}_m , respectively. Then, the Folklore Lemma tells us that

$$\mathbf{D}(\mathbb{X}_n) \sim_{perm} \mathbf{D}(\mathbb{Y}_m)$$

$$\Updownarrow$$

$$\mathbb{X}_n \simeq_{rigid-isom} \mathbb{Y}_m$$

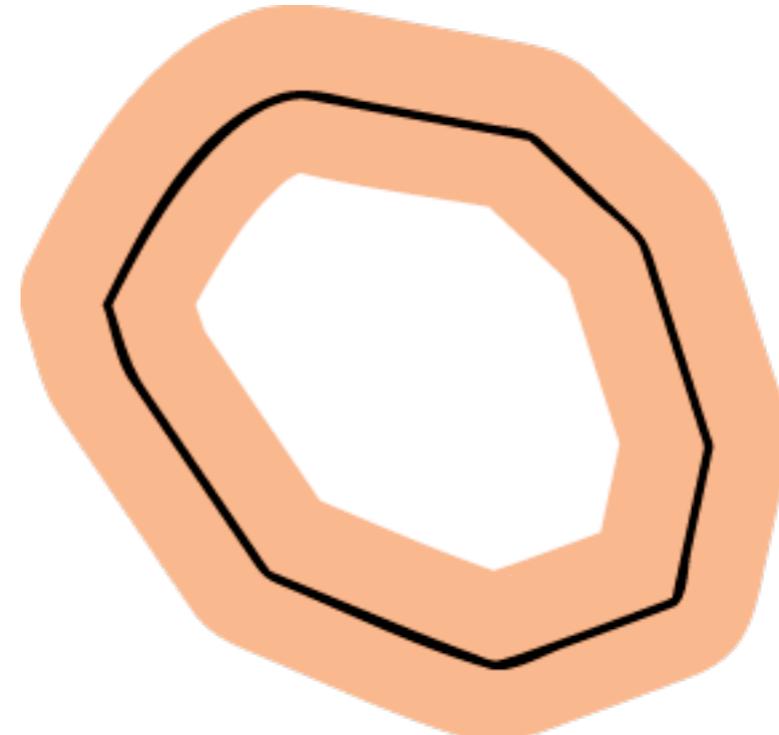
- **Hausdorff distance.** For (compact) subsets A, B of a (compact) metric space (Z, d) , the *Hausdorff distance* between them, $d_{\mathcal{H}}^Z(A, B)$, is defined to be the infimal $\varepsilon > 0$ s.t.

$$A \subset B^\varepsilon$$

and

$$B \subset A^\varepsilon$$

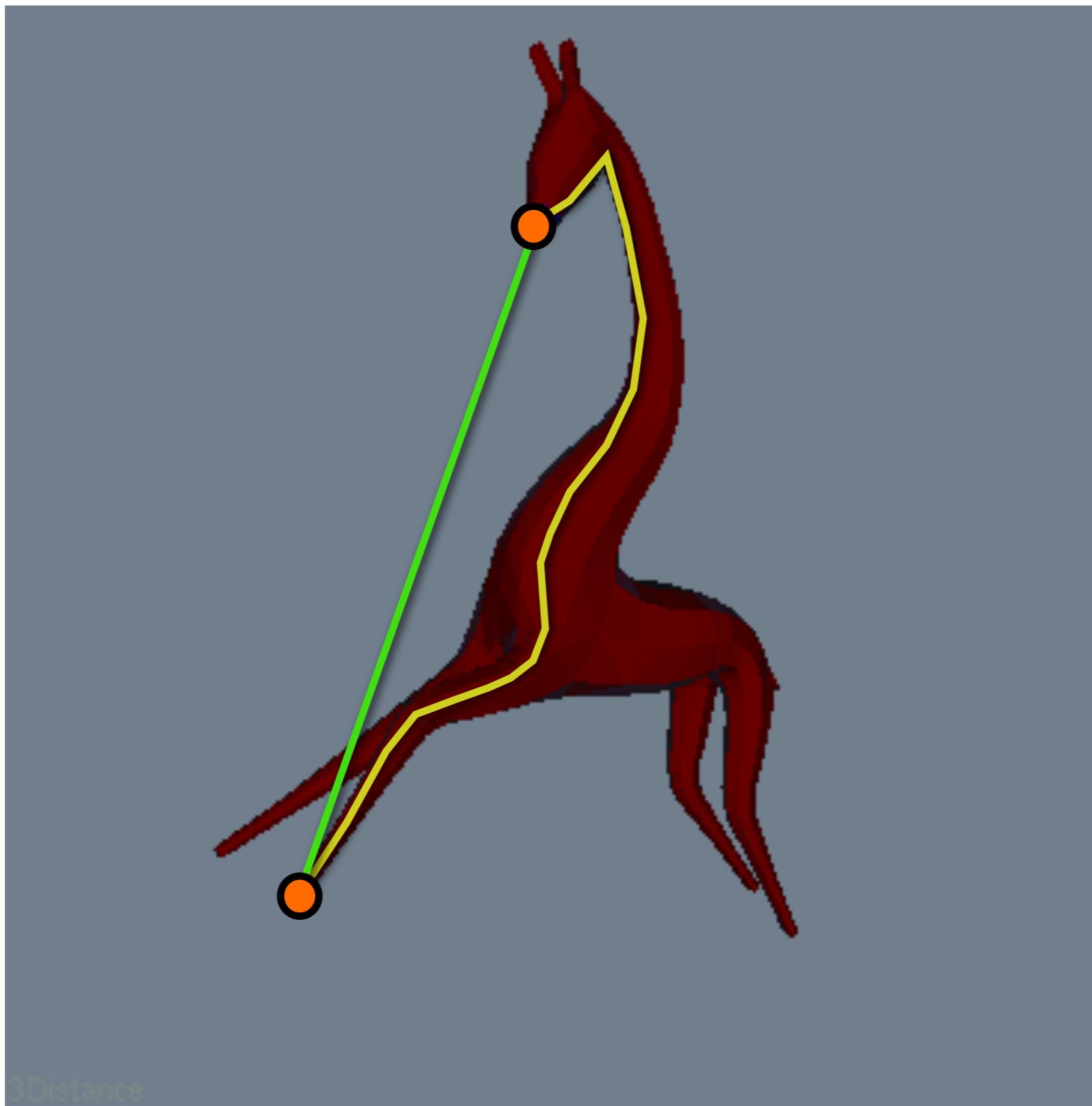
where $A^\varepsilon = \{z \in Z \mid d(z, A) < \varepsilon\}$.



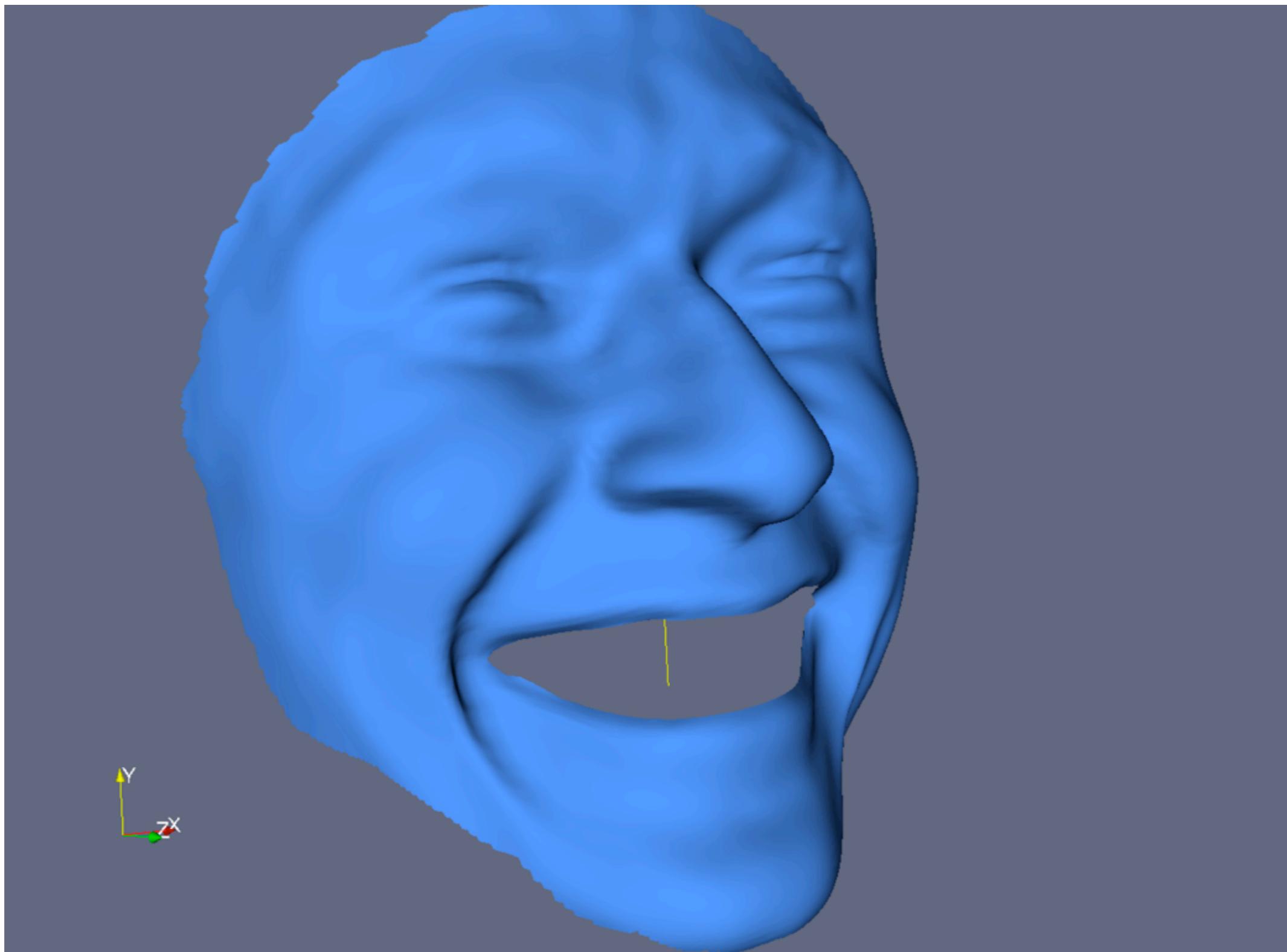
Equivalently,

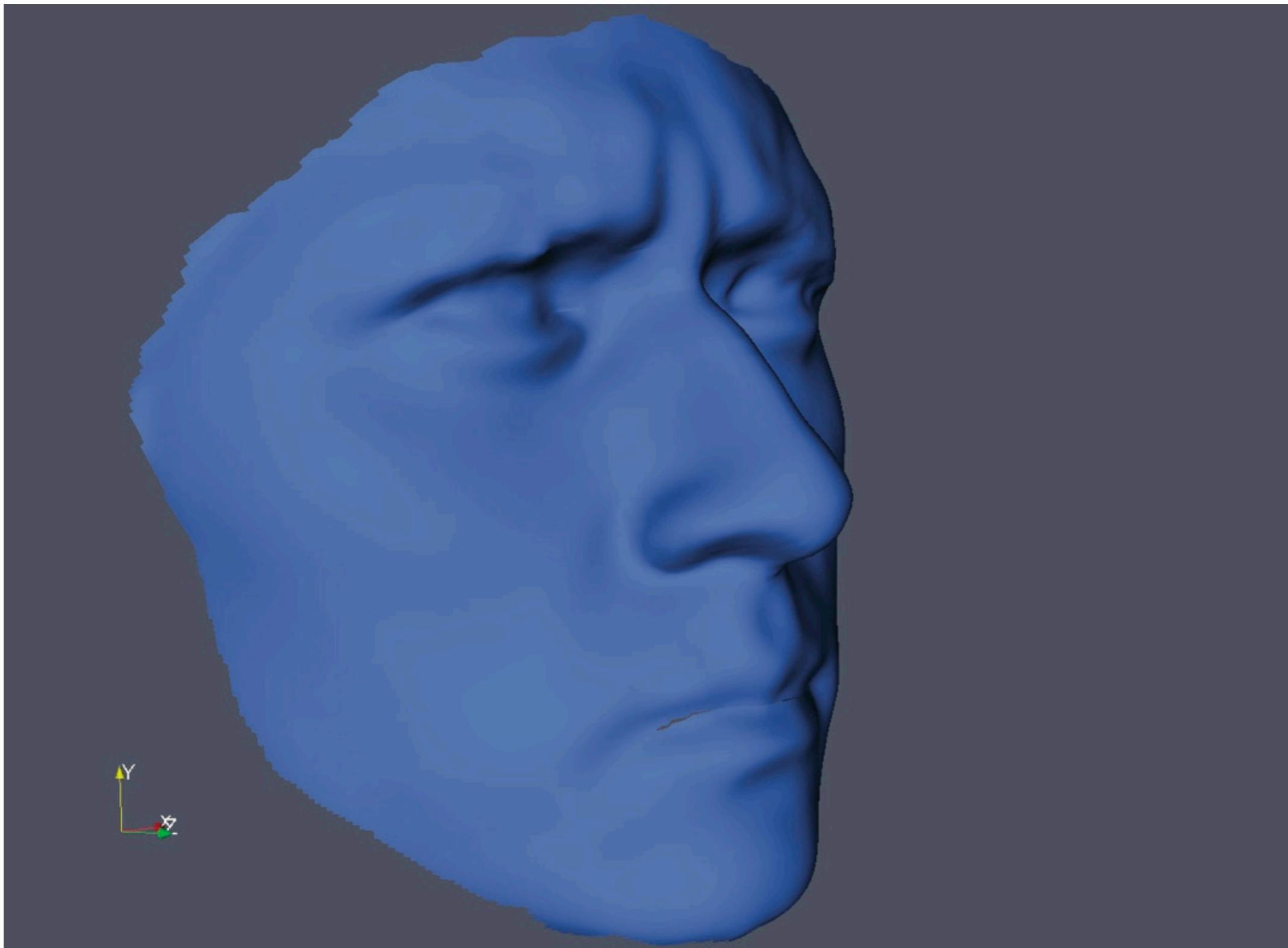
$$d_{\mathcal{H}}^Z(A, B) = \max\left(\max_{b \in B} \min_{a \in A} d(a, b), \max_{a \in A} \min_{b \in B} d(a, b)\right)$$

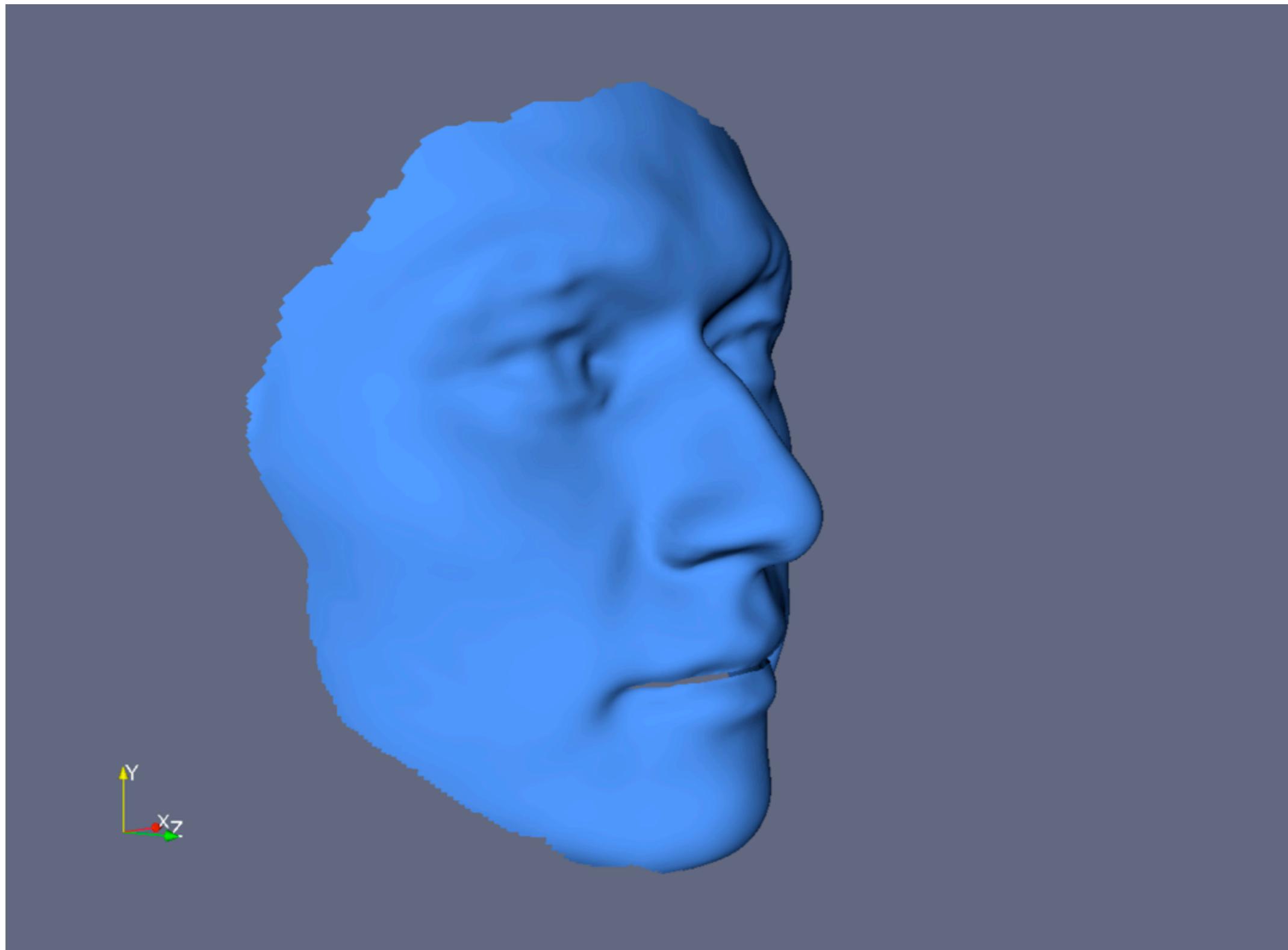
Geodesic distance vs Euclidean distance

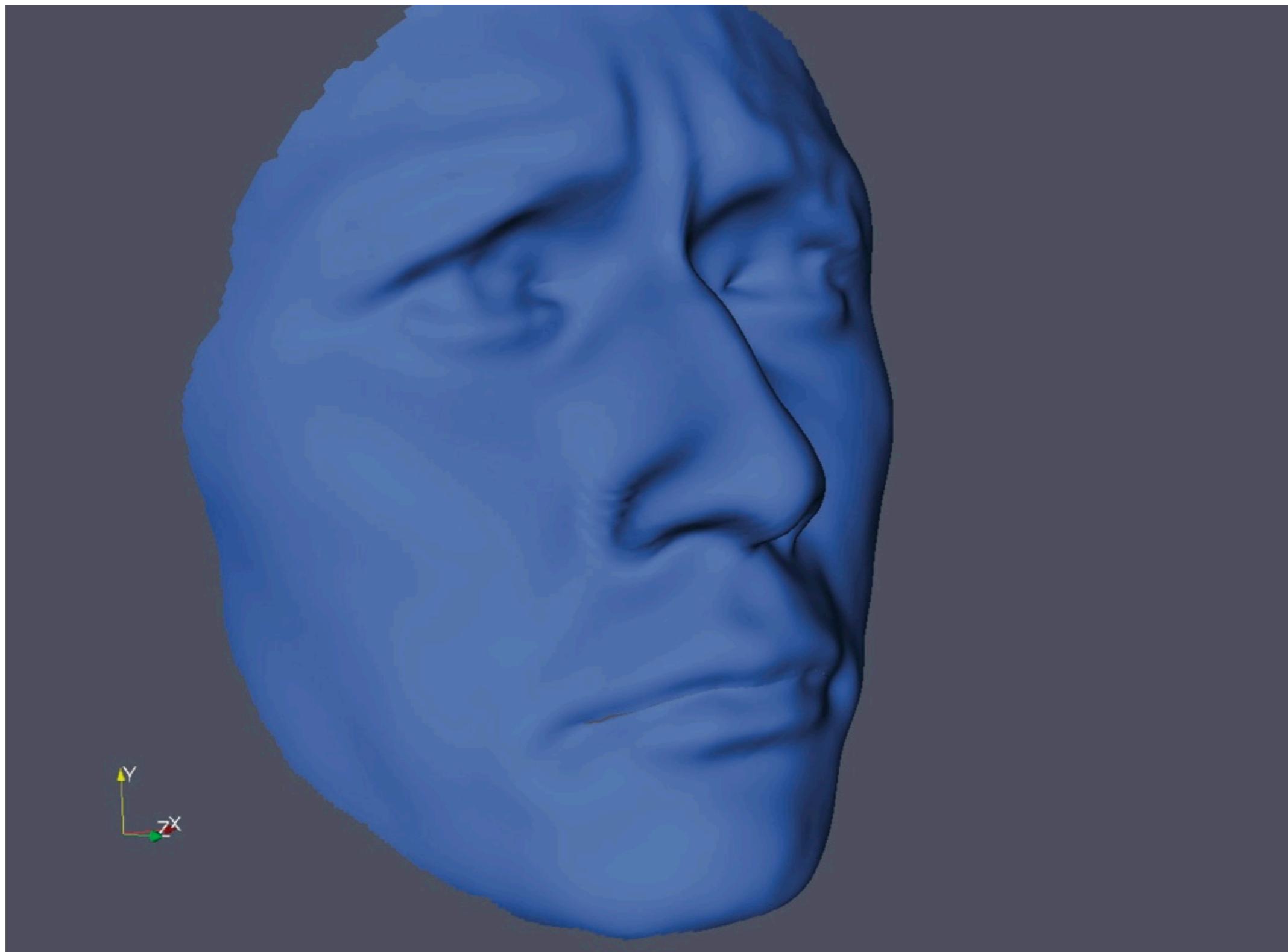


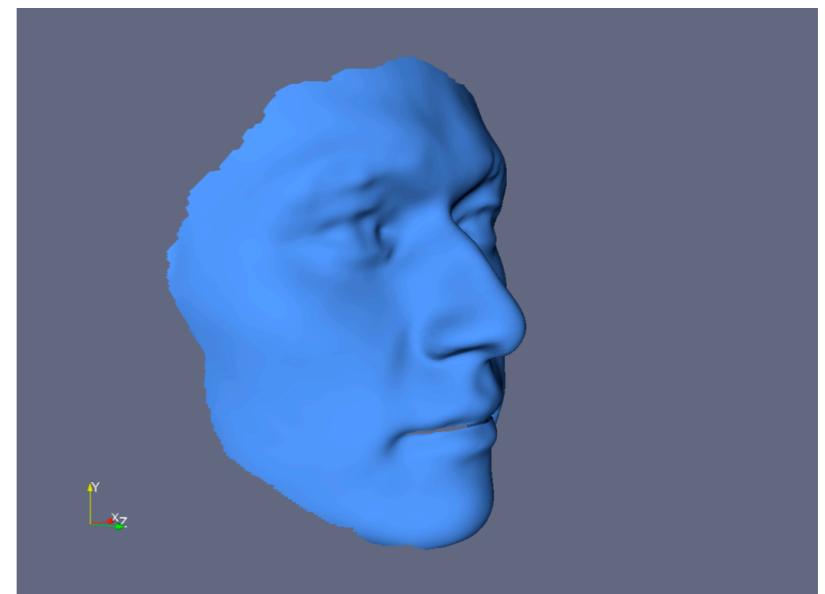
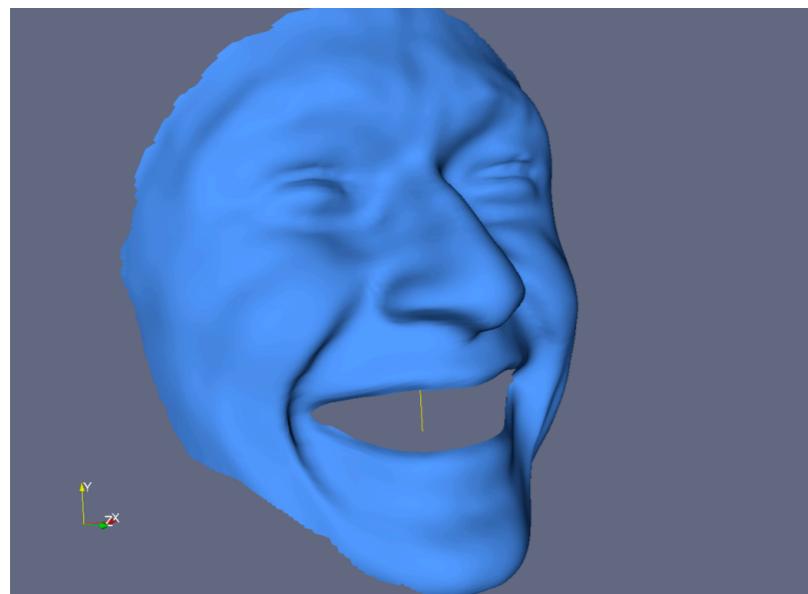
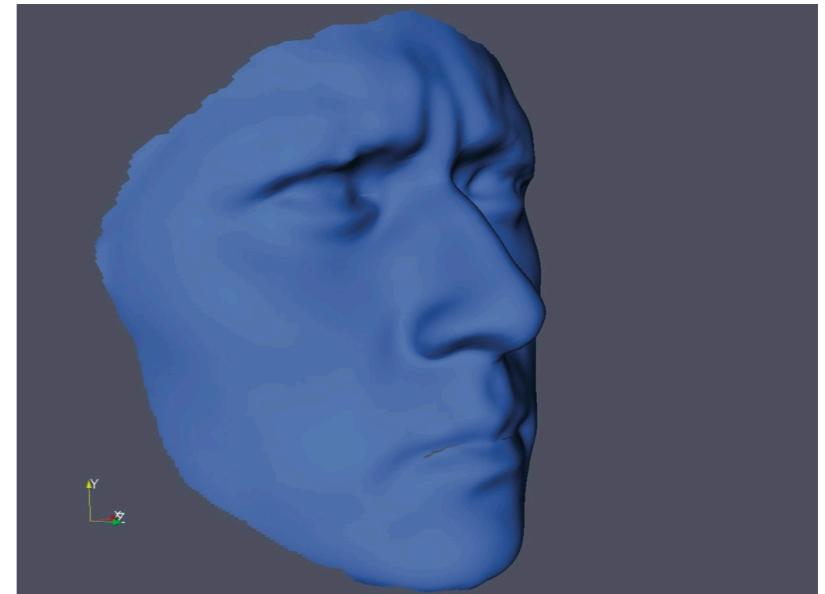
Geodesic distance: invariance to ‘bends’

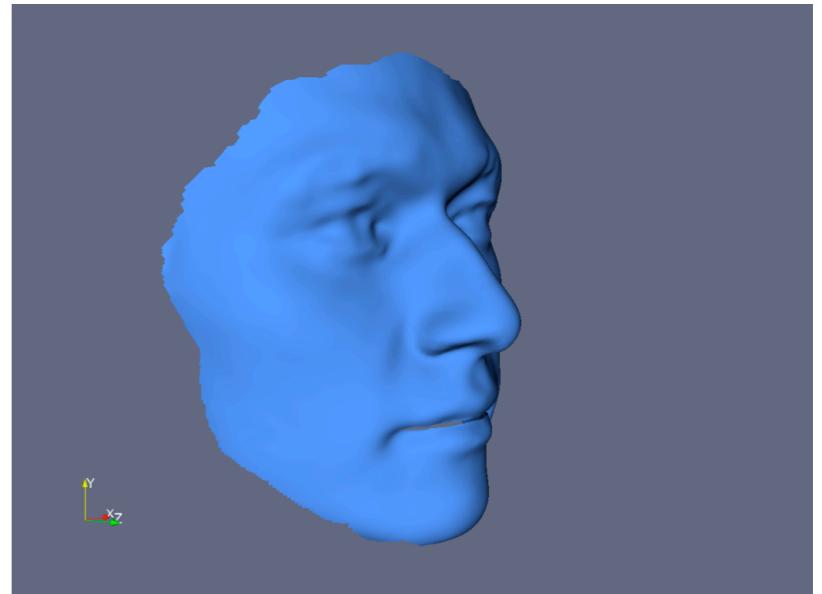
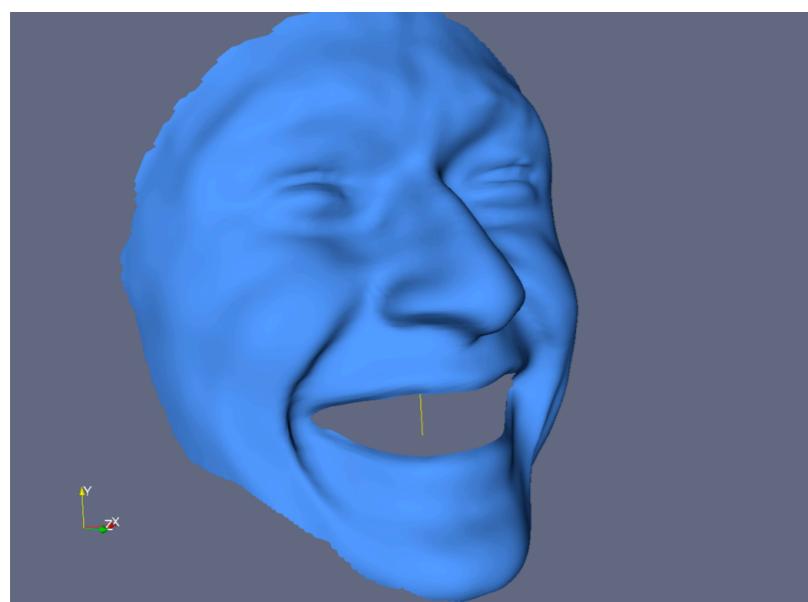
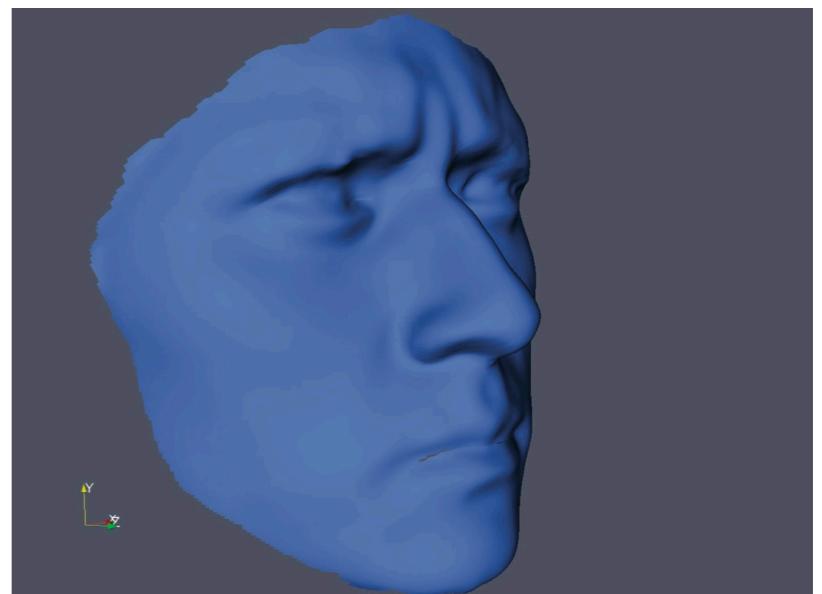


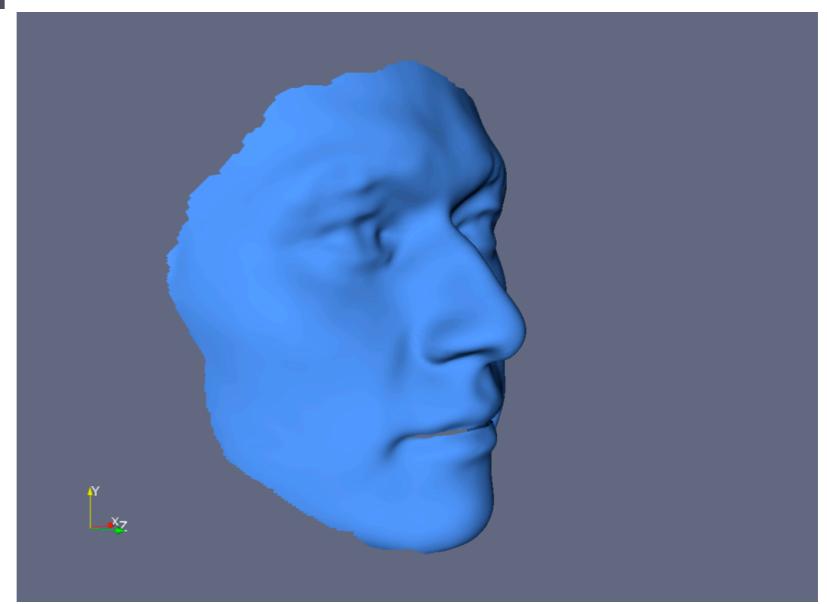
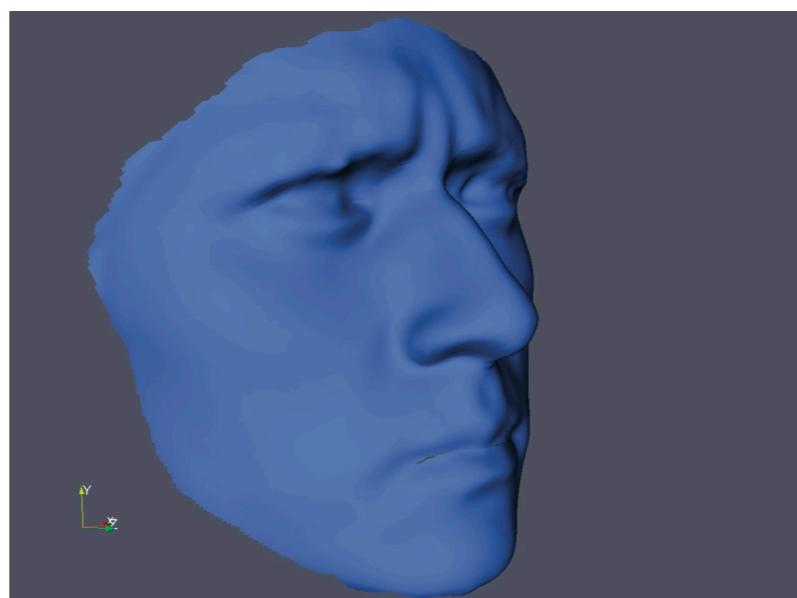
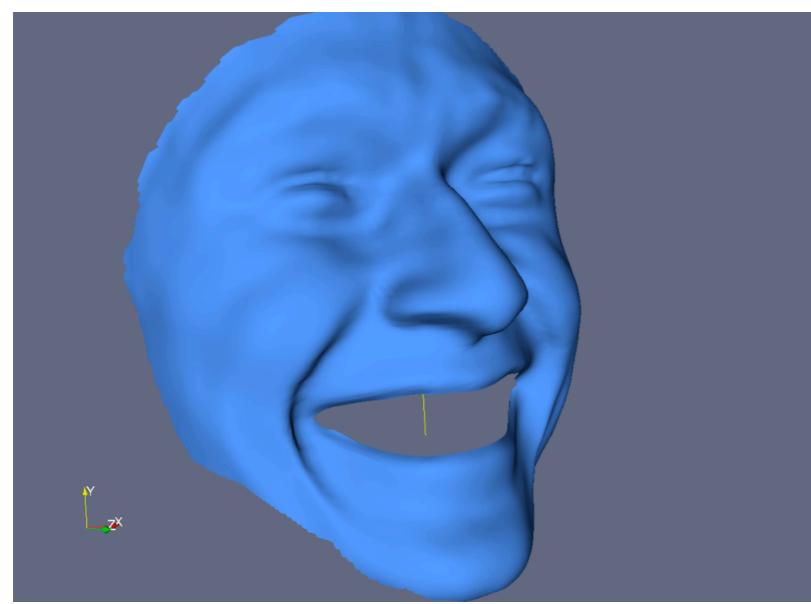


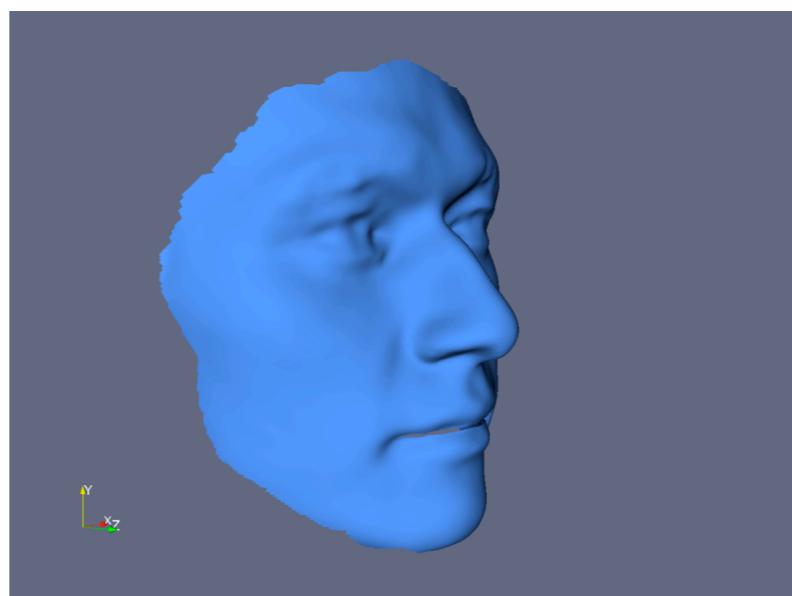
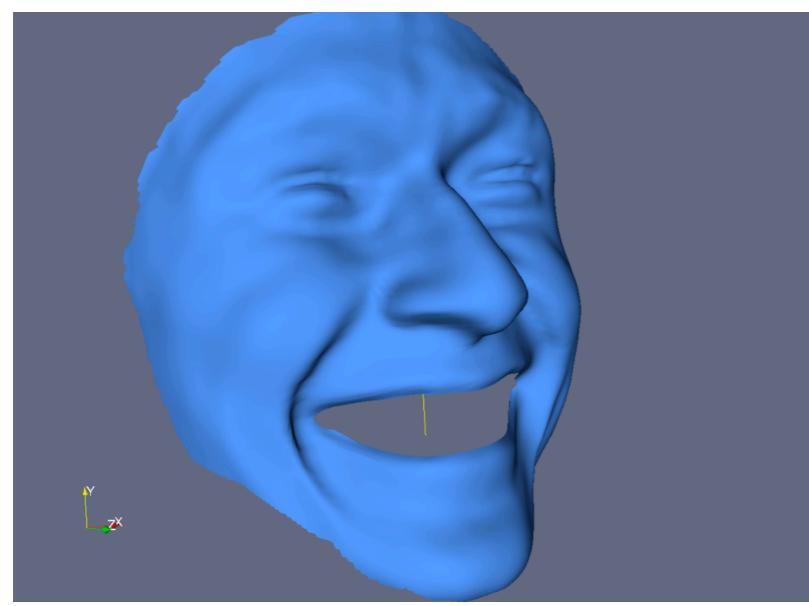


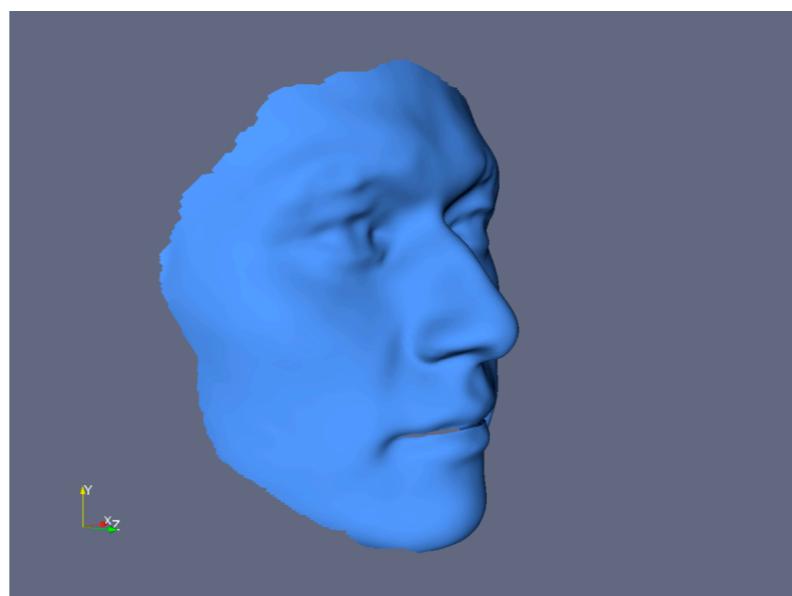






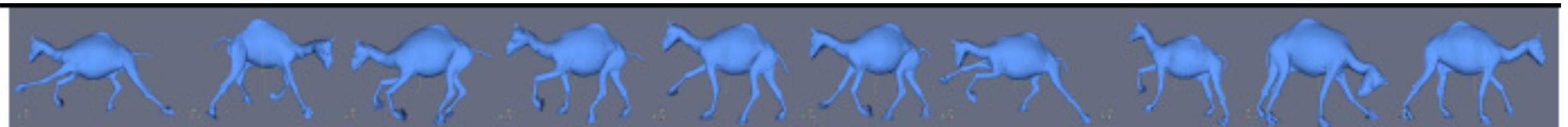






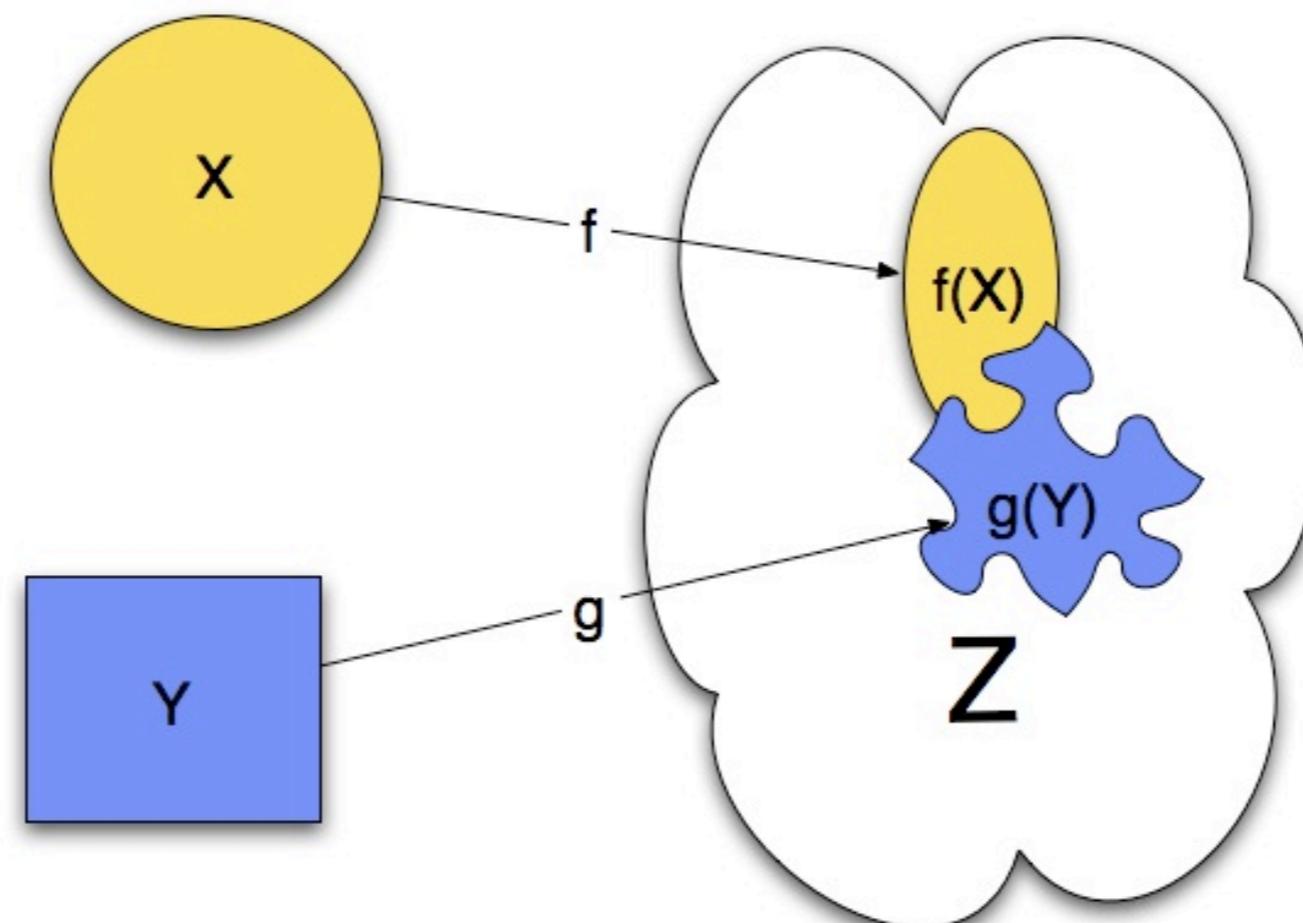
The GH distance for Shape Comparison

- Regard shapes as (compact) metric spaces, [MS04], [MS05].
- The metric with which one endows the shapes depends on the desired invariance. For example, if invariance to
 - *rigid isometries* is desired, use Euclidean distance (remember Folklore Lemma).
 - *bends* is desired, use "geodesic" distance.
- Let \mathcal{X} denote set of all compact metric spaces. Define GH distance (metric) on \mathcal{X} , then (\mathcal{X}, d_{GH}) is itself a metric space.
- GH distance provides reasonable framework for Shape Comparison: good theoretical properties.
- However, it leads to difficult optimization problems.



GH: definition

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



It would be much more intuitive to compare the metrics d_X and d_Y directly..

For maps $f : X \rightarrow Y$, and $g : Y \rightarrow X$ compute

$$\text{dist}(f) = \max_{x,x'} |d_X(x, x') - d_Y(f(x), f(x'))|$$

and

$$\text{dist}(g) = \max_{y,y'} |d_Y(y, y') - d_X(g(y), g(y'))|$$

and then minimize $\max(\text{dist}(f), \text{dist}(g))$ over all choices of f and g .

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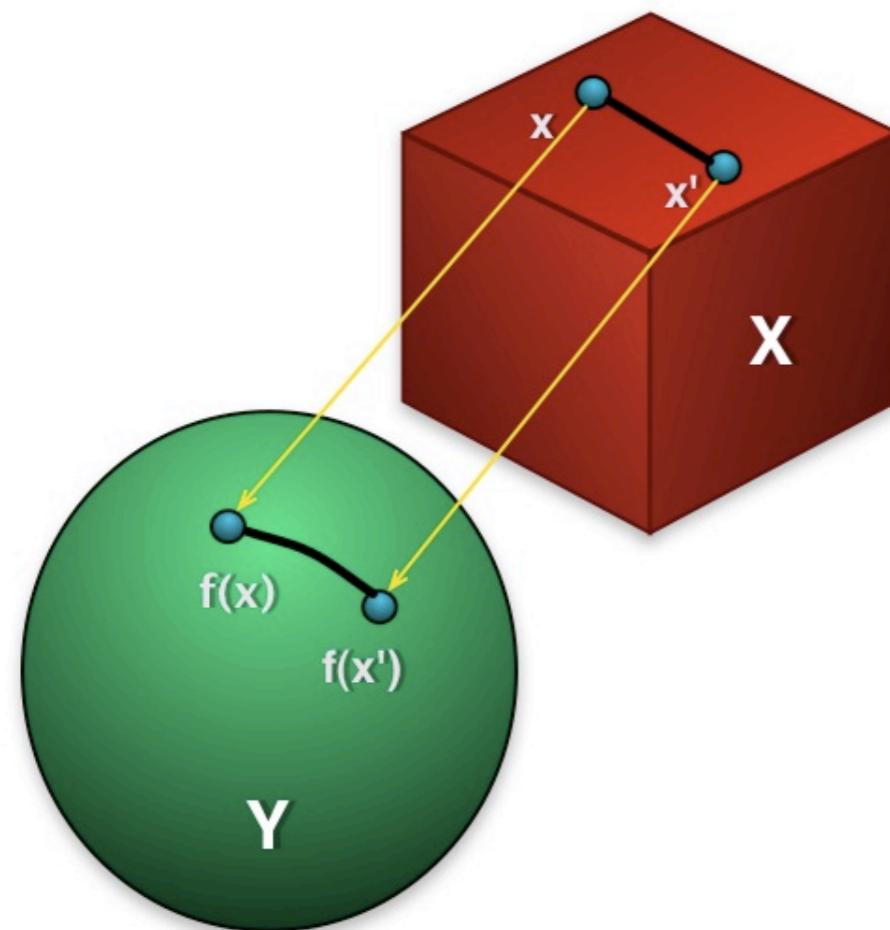
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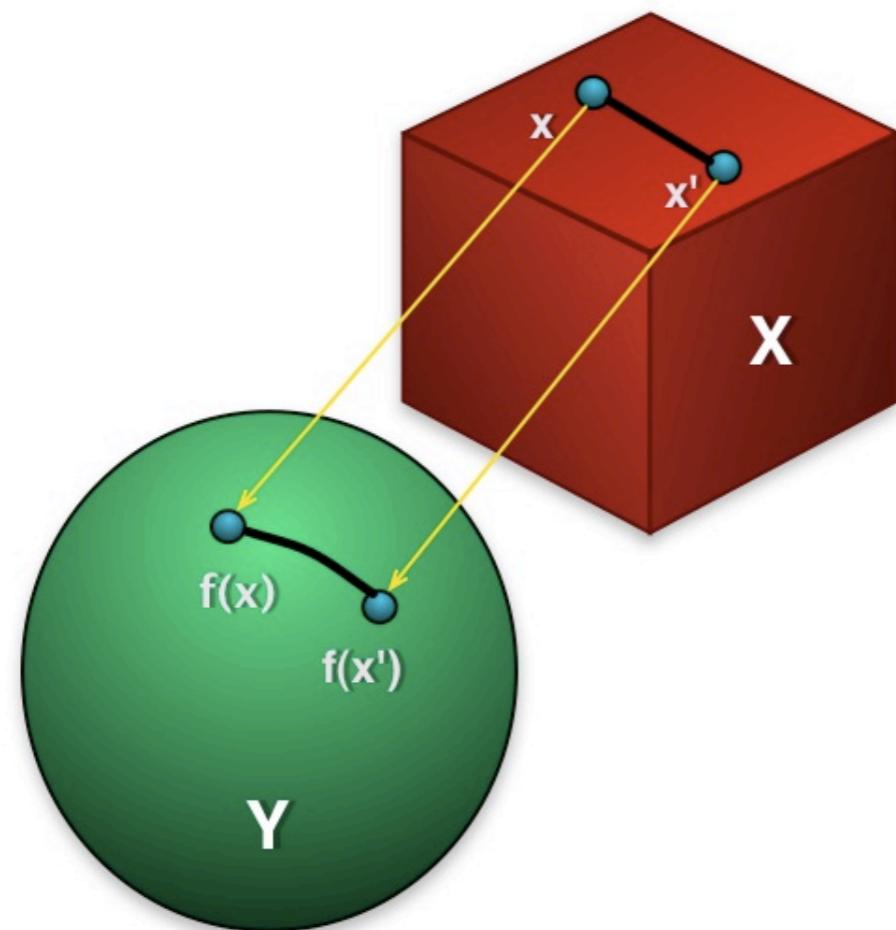
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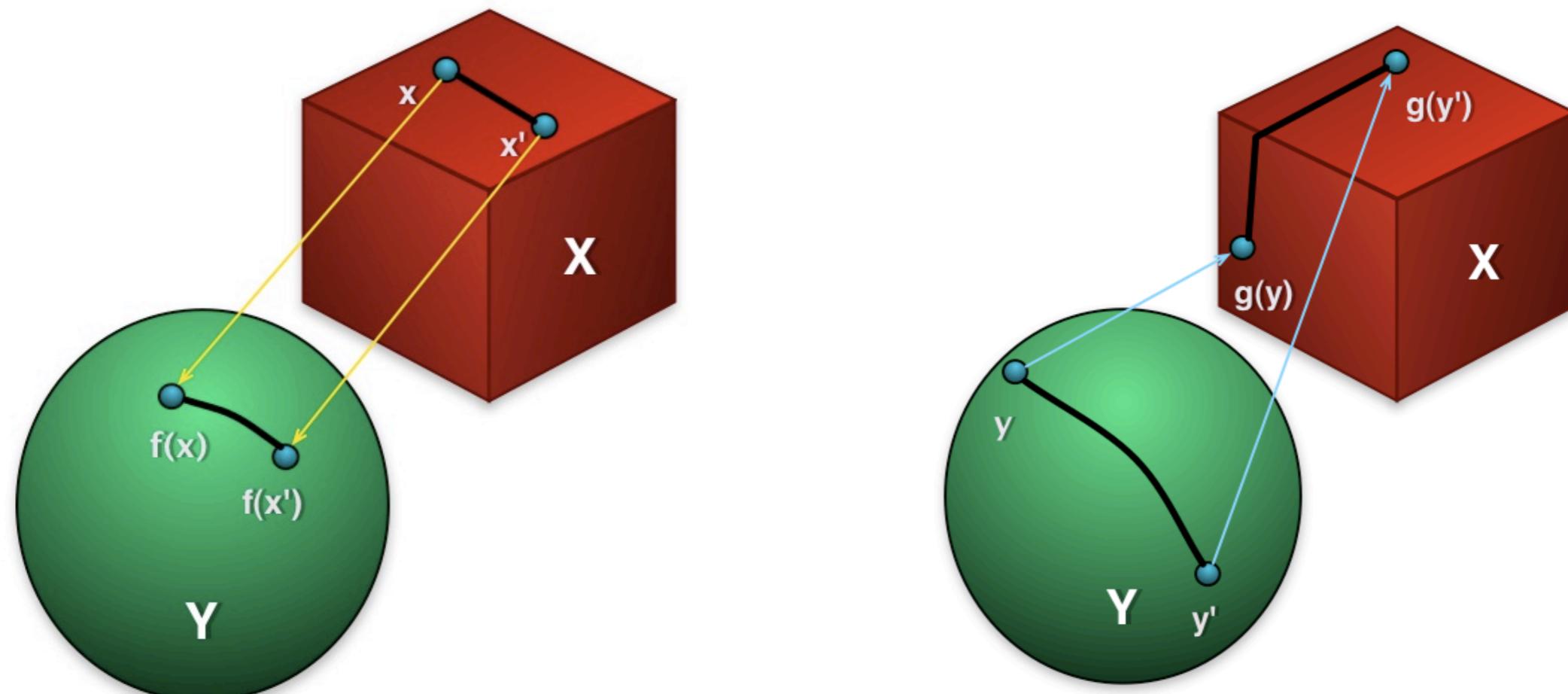
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correspondences

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.

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

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

		B						
		0	1	1	0	0	1	1
		1	1	0	1	0	1	1
		1	0	1	0	1	1	0
		0	0	0	0	0	0	0
		1	0	1	1	0	1	0

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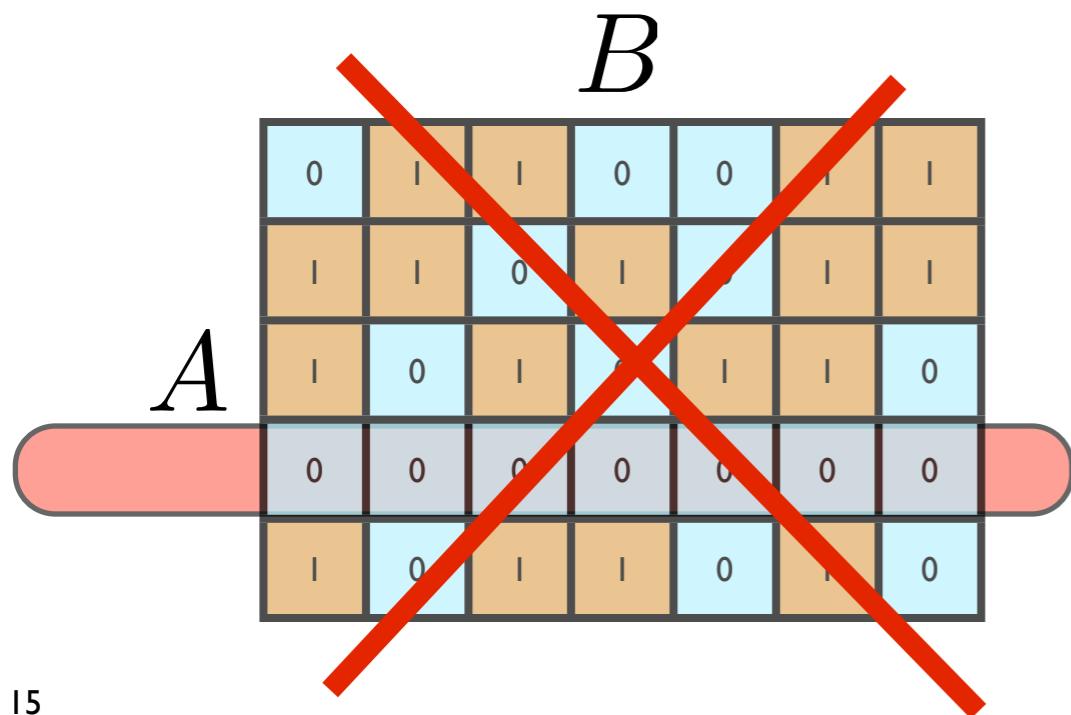
B							
A	0	1	1	0	0	1	1
	1	1	0	1	0	1	1
	1	0	1	0	1	1	0
	0	0	0	0	0	0	0
	1	0	1	1	0	1	0

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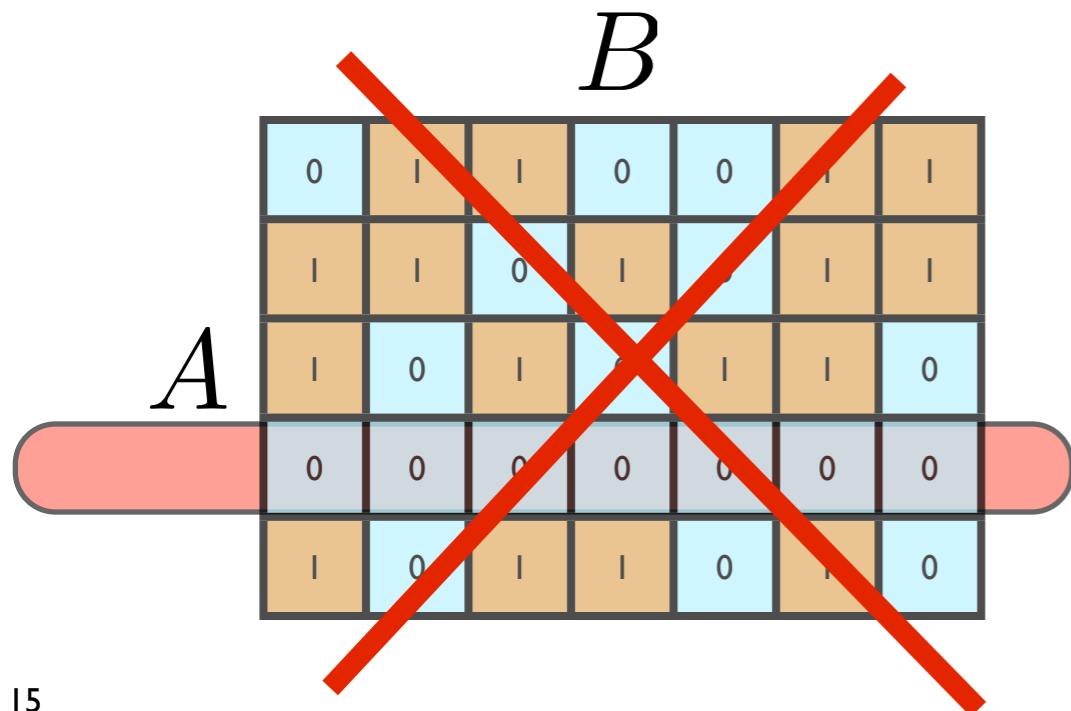


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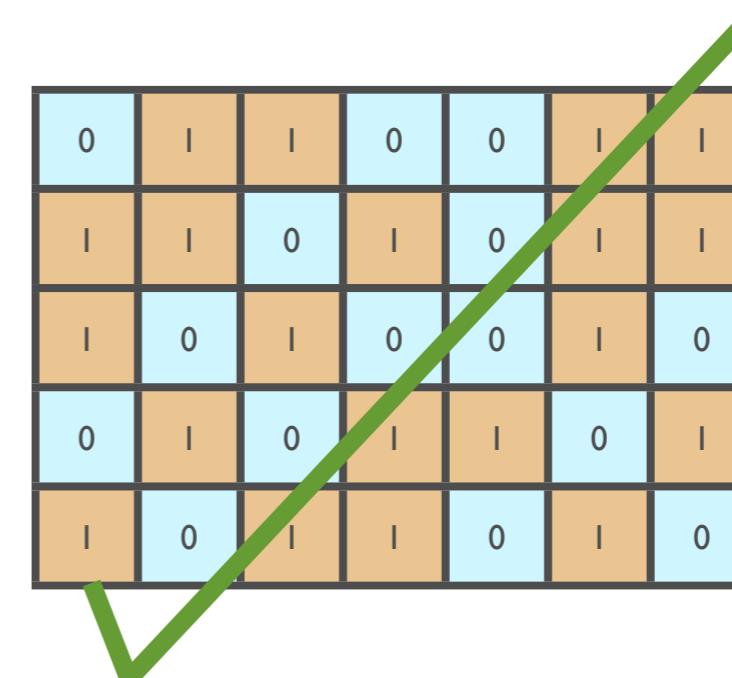
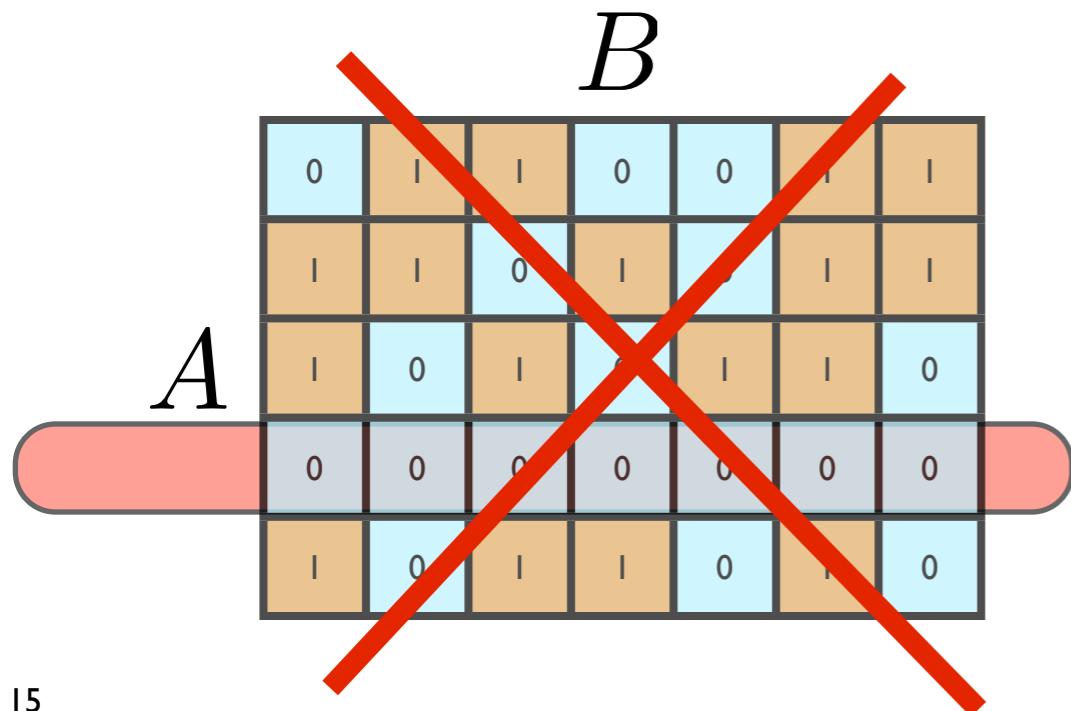
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1	1	0	1	1	1	1
1	0	1	1	1	1	0
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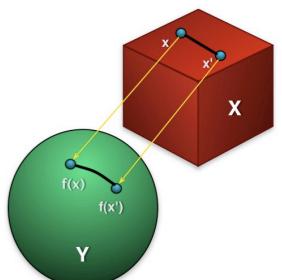


Another expression for the GH distance

A theorem, [BuBuIv]

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

$$d_{\mathcal{H}}(X, Y) = \frac{1}{2} \inf_R \max_{(\textcolor{red}{x}, \textcolor{red}{y}), (\textcolor{blue}{x}', \textcolor{blue}{y}') \in R} |d_X(\textcolor{red}{x}, \textcolor{blue}{x}') - d_Y(\textcolor{red}{y}, \textcolor{blue}{y}')|$$



Main Properties

1. Let (X, d_X) , (Y, d_Y) and (Z, d_Z) be metric spaces then

$$d_{\mathcal{GH}}(X, Y) \leq d_{\mathcal{GH}}(X, Z) + d_{\mathcal{GH}}(Y, Z).$$

2. If $d_{\mathcal{GH}}(X, Y) = 0$ and (X, d_X) , (Y, d_Y) are compact metric spaces, then (X, d_X) and (Y, d_Y) are isometric.
3. Let $\mathbb{X}_n = \{x_1, \dots, x_n\} \subset X$ be a finite subset of the compact metric space (X, d_X) . Then,

$$d_{\mathcal{GH}}(X, \mathbb{X}_n) \leq d_{\mathcal{H}}(X, \mathbb{X}_n).$$

4. For compact metric spaces (X, d_X) and (Y, d_Y) :

$$\begin{aligned} \frac{1}{2} |\text{diam}(X) - \text{diam}(Y)| &\leq d_{\mathcal{GH}}(X, Y) \\ &\leq \frac{1}{2} \max(\text{diam}(X), \text{diam}(Y)) \end{aligned}$$

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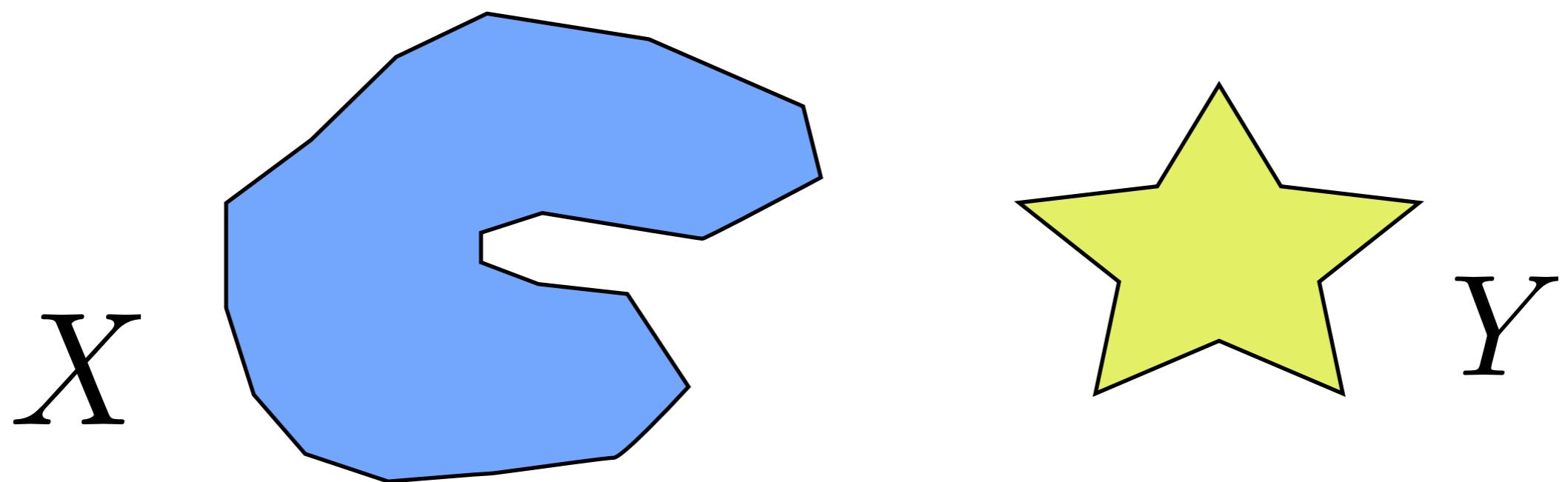
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Stability, [MS05]

$$|d_{\mathcal{GH}}(X, Y) - d_{\mathcal{GH}}(\mathbb{X}_n, \mathbb{Y}_m)| \leq r(\mathbb{X}_n) + r(\mathbb{Y}_m)$$

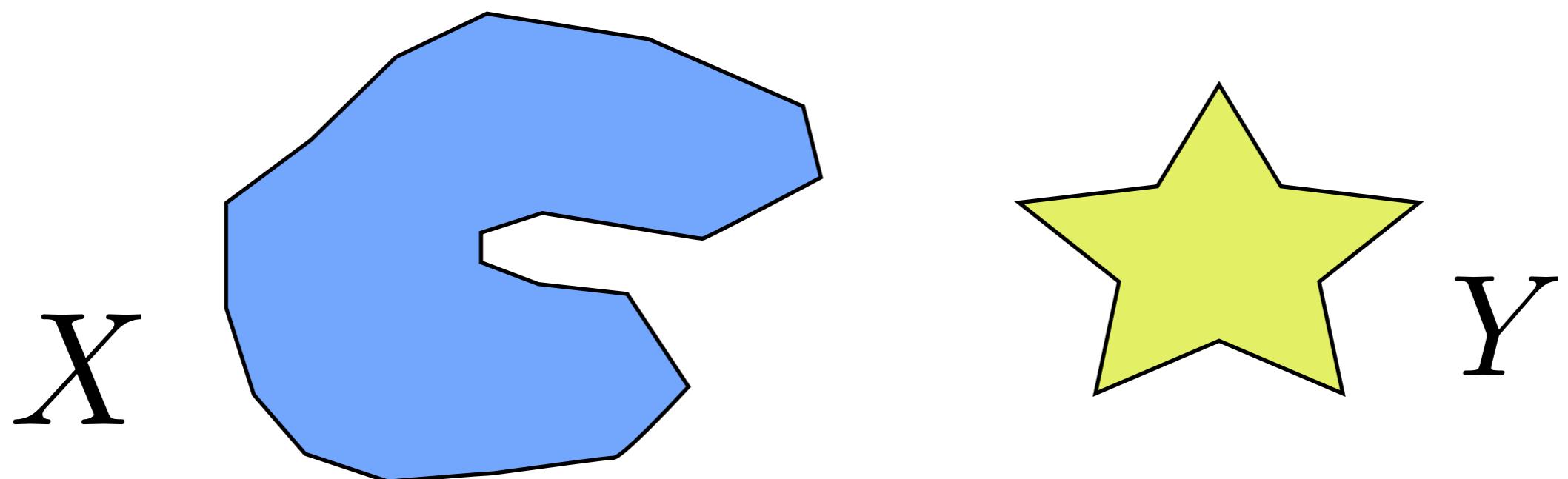
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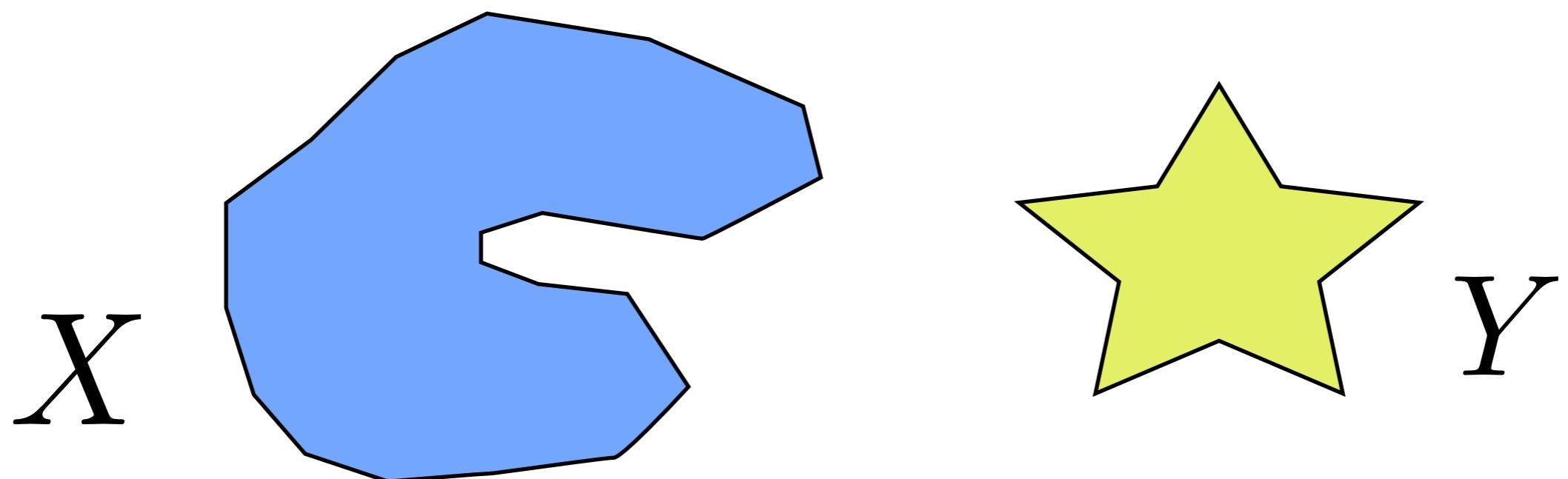
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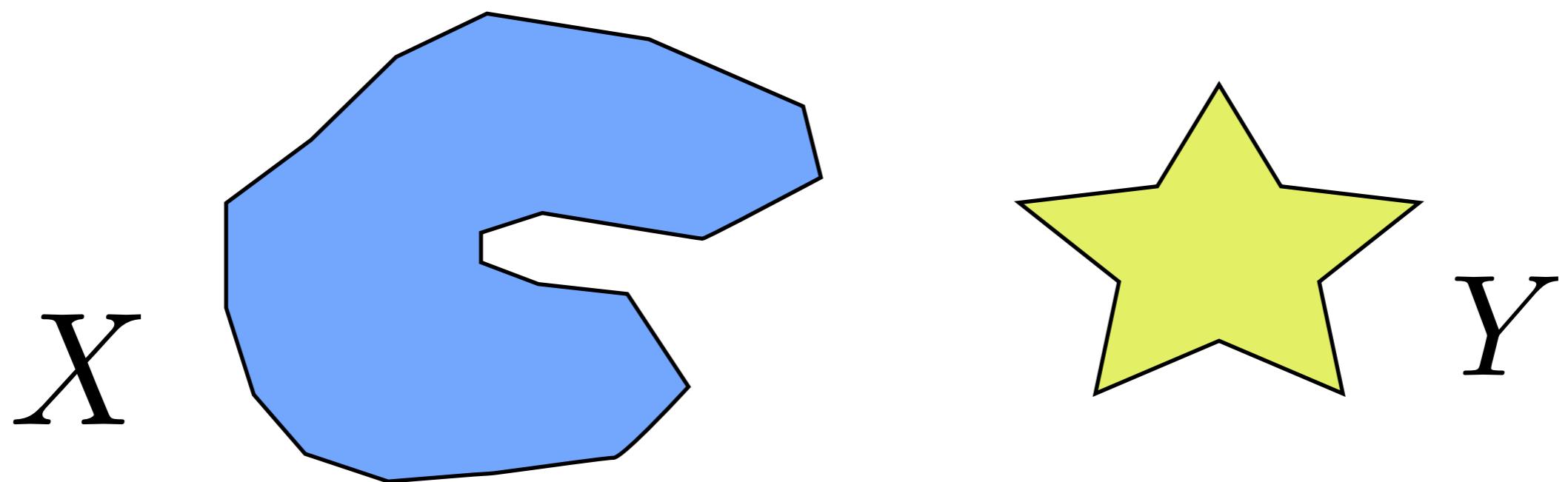
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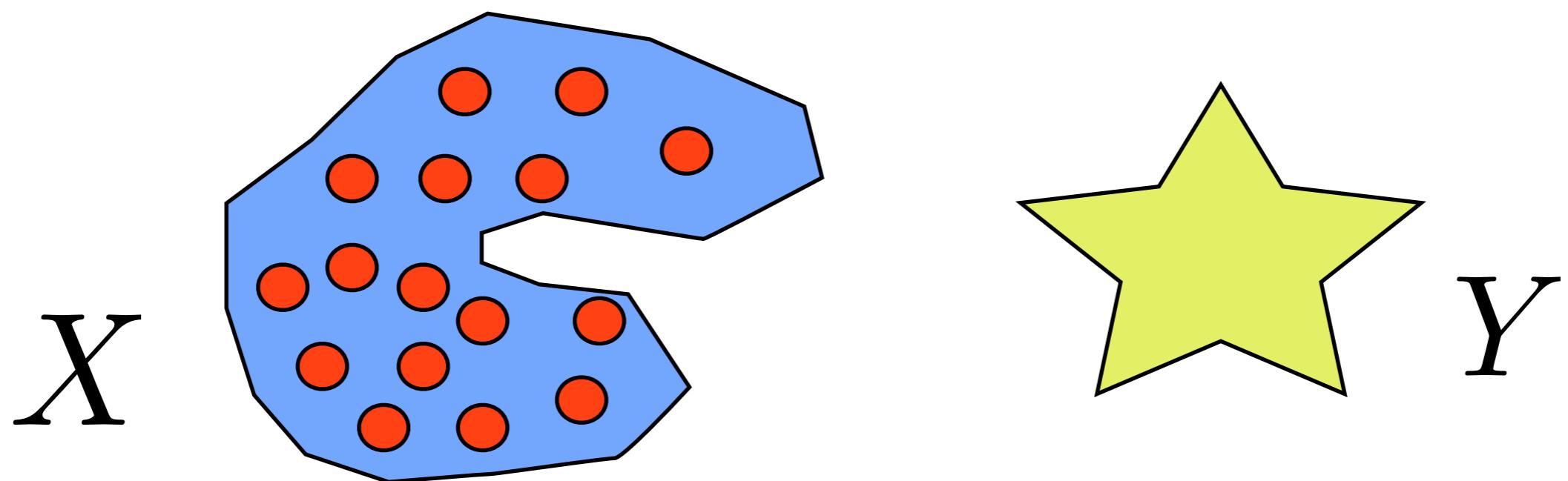
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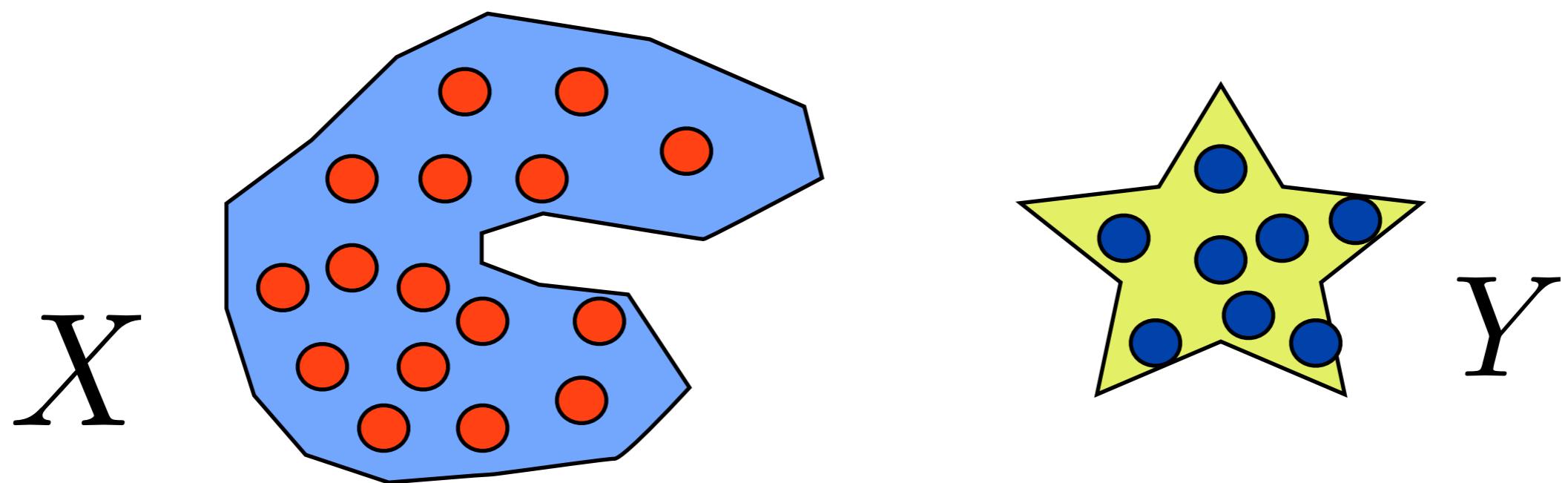
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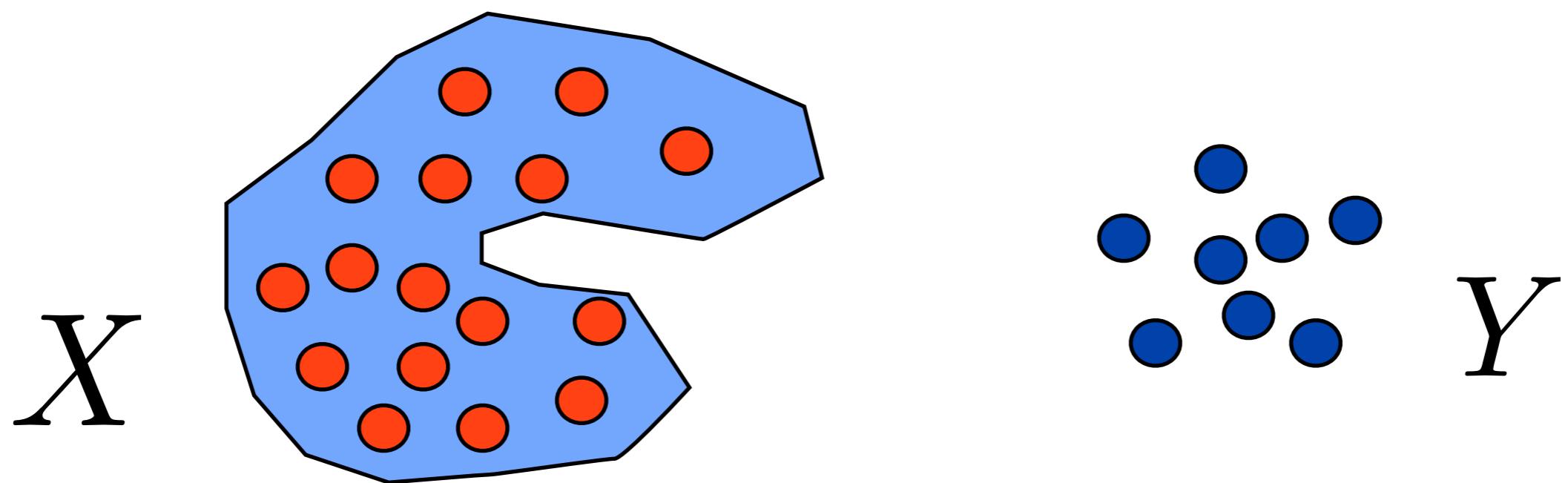
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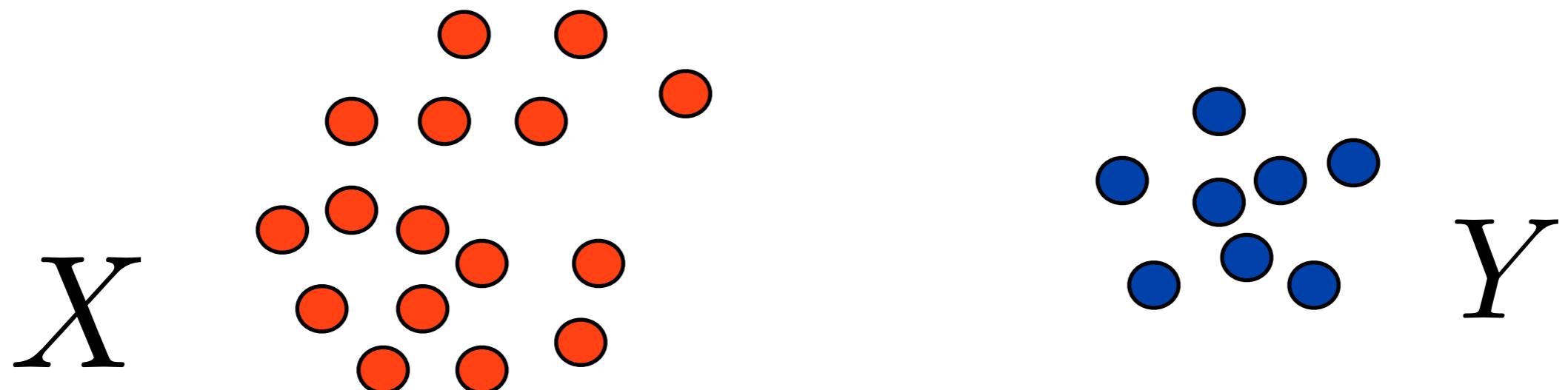
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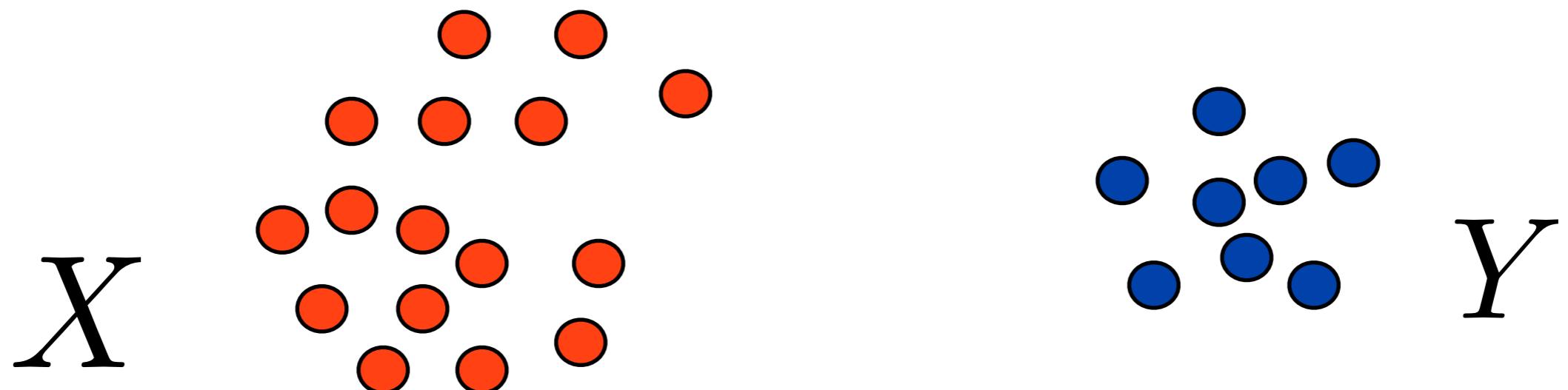
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Critique

- Was not able to show connections with (sufficiently many) pre-existing approaches such as Shape Distributions, Shape Contexts, Hamza-Krim, Frosini et al.
- Computationally hard: currently only two attempts have been made:
 - [MS04,MS05] and [BBK06] only for surfaces.
 - [MS05] gives probabilistic guarantees for estimator based on sampling parameters.
 - Full generality leads to a hard **combinatorial optimization problem**: QAP.

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- Computationally hard: currently only two attempts have been made:
 - [MS04,MS05] and [BBK06] only for surfaces.
 - [MS05] gives probabilistic guarantees for estimator based on sampling parameters.
 - Full generality leads to a hard **combinatorial optimization problem**: QAP.

Desiderata

- Obtain an L^p version of the GH distance that:
 - retains theoretical underpinnings
 - its implementation leads to easier (continuous, quadratic, with linear constraints) optimization problems
 - can be related to pre-existing approaches (shape contexts, shape distributions, Hamza-Krim,...) via lower/upper bounds.

First attempt: naive relaxation

Remember that

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

where $R \in \mathcal{R}(X, Y)$. Using the matricial representation of R one can write

$$d_{\mathcal{GH}}(X, Y) = \frac{1}{2} \inf_R \max_{\textcolor{red}{x}, \textcolor{blue}{x}', \textcolor{red}{y}, \textcolor{blue}{y}'} |d_X(\textcolor{red}{x}, \textcolor{blue}{x}') - d_Y(\textcolor{red}{y}, \textcolor{blue}{y}')| r_{\textcolor{red}{x}, \textcolor{red}{y}} r_{\textcolor{blue}{x}', \textcolor{blue}{y}'}$$

where $R = ((r_{x,y})) \in \{0, 1\}^{n_X \times n_B}$ s.t.

$$\sum_{x \in X} r_{xy} \geq 1 \quad \forall y \in Y$$

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First attempt: naive relaxation (continued)

- The idea would be to use L^p norm instead of L^∞ (max max)
- relax $r_{x,y}$ to be in $[0, 1]$ (!)

Then, the idea would be to compute (for some $p \geq 1$):

$$\widehat{d}_{\mathcal{GH}}(X, Y) = \frac{1}{2} \inf_R \left(\sum_{\textcolor{red}{x}, \textcolor{blue}{x}', \textcolor{red}{y}, \textcolor{blue}{y}'} |d_X(\textcolor{red}{x}, \textcolor{blue}{x}') - d_Y(\textcolor{red}{y}, \textcolor{blue}{y}')|^p r_{\textcolor{red}{x}, \textcolor{red}{y}} r_{\textcolor{blue}{x}', \textcolor{blue}{y}'} \right)^{1/p}$$

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- The resulting problem is a continuous variable QOP with linear constraints, but..
- there is no limit problem.. this discretization cannot be connected to the GH distance..

we need to identify the **correct** relaxation of the GH distance. More precisely, the correct notion of *relaxed correspondence*.

More background

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

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.



correspondences and measure couplings

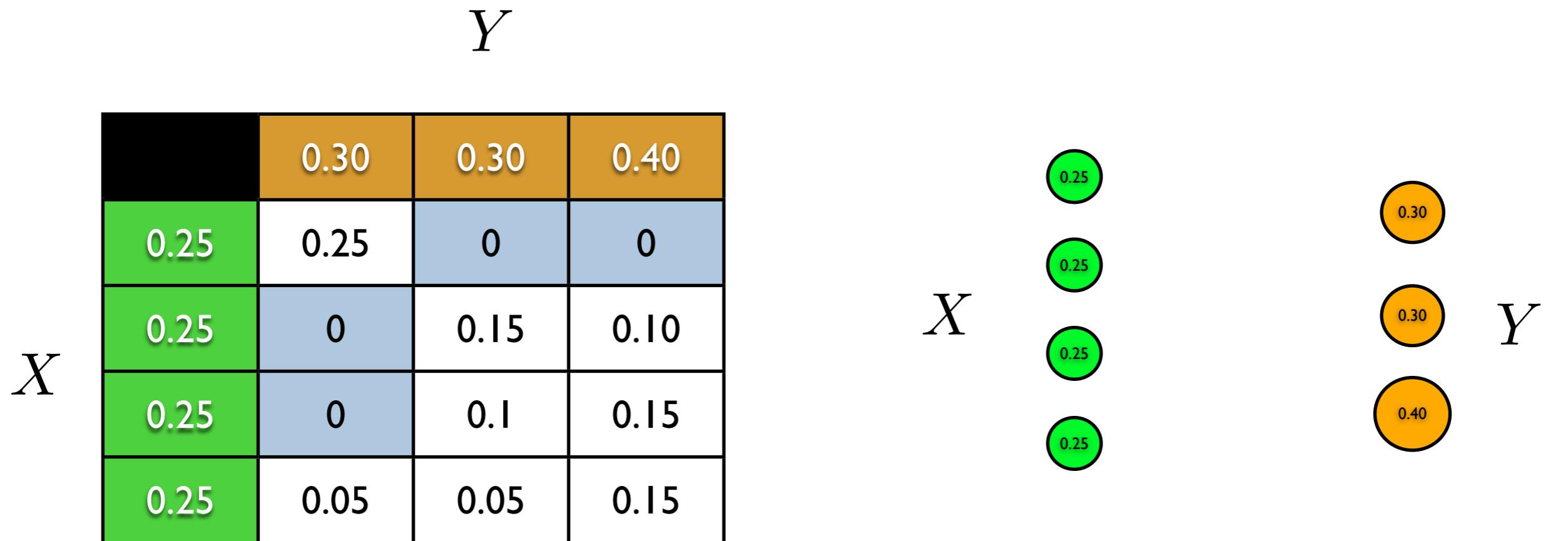
Let A and B be compact subsets of the compact metric space (X, d) and μ_A and μ_B be **probability measures** supported in A and B respectively.

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

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

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.



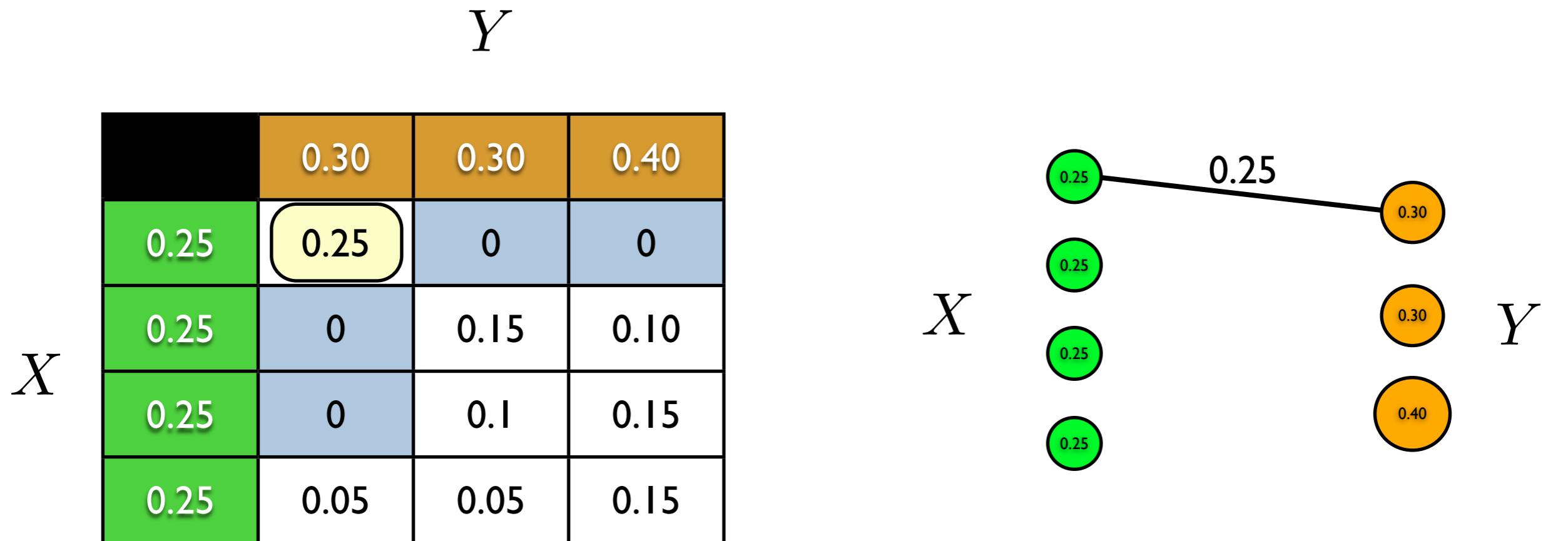
The support of the coupling consists of the non-zero entries.

Y

	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

 X X  Y

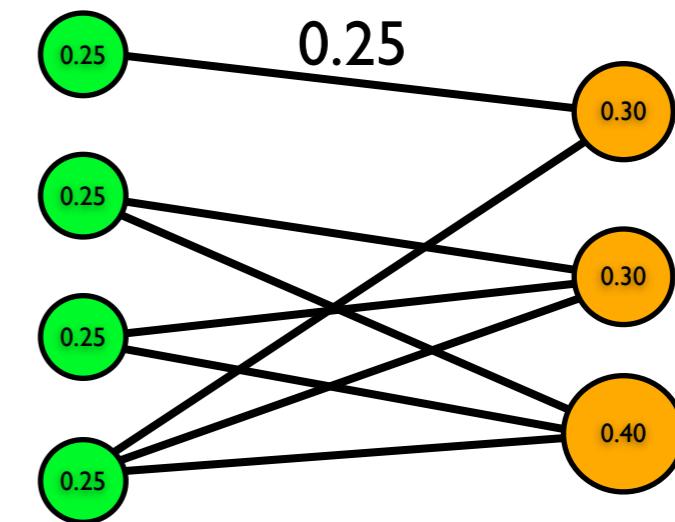
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L^p Gromov-Hausdorff distances [M07]

Compute (for some $p \geq 1$):

$$\mathbf{D}_p(X, Y) = \frac{1}{2} \inf_{\mu} \left(\sum_{\textcolor{red}{x}, \textcolor{blue}{x'}, \textcolor{red}{y}, \textcolor{blue}{y'}} |d_X(\textcolor{red}{x}, \textcolor{blue}{x'}) - d_Y(\textcolor{red}{y}, \textcolor{blue}{y'})|^p \mu_{\textcolor{red}{x}, \textcolor{red}{y}} \mu_{\textcolor{blue}{x'}, \textcolor{blue}{y'}} \right)^{1/p}$$

where $\mu = ((\mu_{x,y})) \in [0, 1]^{n_X \times n_Y}$ s.t.

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This is a QOP with linear constraints! Also, thanks to concepts from measure theory, there is a continuous counterpart (sampling theory)

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This is a QOP with linear constraints! Also, thanks to concepts from measure theory, there is a continuous counterpart (sampling theory)

Numerical Implementation

- The numerical implementation of the second option leads to solving a continuous variable **QOP** with linear constraints:

$$\begin{aligned} & \min_U \frac{1}{2} U^T \boldsymbol{\Gamma} U \\ \text{s.t. } & U_{ij} \in [0, 1], U\mathbf{A} = \mathbf{b} \end{aligned}$$

where $U \in \mathbb{R}^{n_X \times n_Y}$ is the *unrolled* version of μ , $\boldsymbol{\Gamma} \in \mathbb{R}^{n_X \times n_Y \times n_X \times n_Y}$ is the unrolled version of $\Gamma_{X,Y}$ and \mathbf{A} and \mathbf{b} encode the linear constraints $\mu \in \mathcal{M}(\mu_X, \mu_Y)$.

- This can be approached for example via gradient descent. The QOP is non-convex in general!
- Initialization is done via solving one of the several *lower bounds* (discussed ahead). All these lower bounds lead to solving **LOPs**.

Shapes as mm-spaces, [M07]

- 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 $\Phi : X \rightarrow Y$ s.t. $\mu_Y(B) = \mu_X(\Phi^{-1}(B))$ for all (measurable) sets $B \subset Y$.

$$(X, d_X, \mu_X)$$

G H



H



G W



W

Properties of \mathbf{D}_p , [M07]

1. Let X, Y and Z mm-spaces then

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

2. If $\mathbf{D}_p(X, Y) = 0$ if and only if X and Y are isomorphic.
3. Let $\mathbb{X}_n = \{x_1, \dots, x_n\} \subset X$ be a subset of the mm-space (X, d, ν) . Endow \mathbb{X}_n with the metric d and a prob. measure ν_n , then

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

The parameter p is not superfluous

The simplest lower bound one has is based on the triangle inequality plus

$$2 \cdot \mathbf{D}_p(X, \{q\}) = \left(\int_{X \times X} d_X(x, x') \nu(dx) \nu(dx') \right)^{1/p} := \mathbf{diam}_p(X)$$

That is

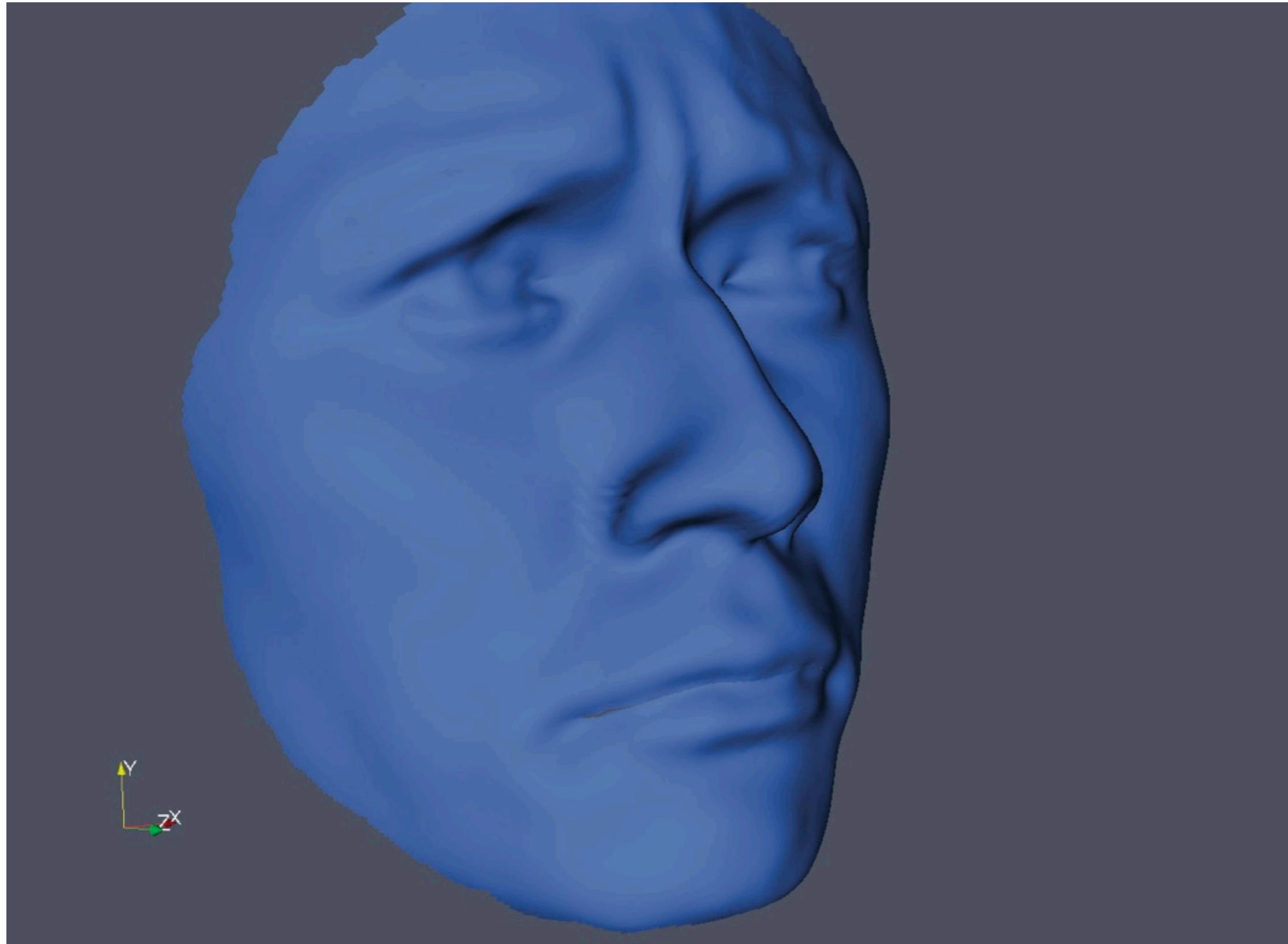
$$\mathbf{D}_p(X, Y) \geq \frac{1}{2} |\mathbf{diam}_p(X) - \mathbf{diam}_p(Y)|$$

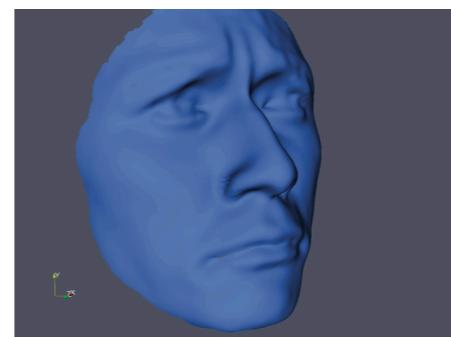
For example, when $X = S^n$ (spheres with uniform measure and usual intrinsic metric):

- $p = \infty$ gives $\mathbf{diam}_\infty(S^n) = \pi$ for all $n \in \mathbb{N}$
- $p = 1$ gives $\mathbf{diam}_1(S^n) = \pi/2$ for all $n \in \mathbb{N}$
- $p = 2$ gives $\mathbf{diam}_2(S^1) = \pi/\sqrt{3}$ and $\mathbf{diam}_2(S^2) = \sqrt{\pi^2/2 - 2}$

Connections with other approaches

- Shape Distributions [**Osada-et-al**]
- Shape contexts [**SC**]
- Hamza-Krim, Hilaga et al approach [**HK**]
- Rigid isometries invariant Hausdorff [**Goodrich**]
- Gromov-Hausdorff distance [**MS04**] [**MS05**]
- Elad-Kimmel idea [**EK**]
- Topology based methods









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

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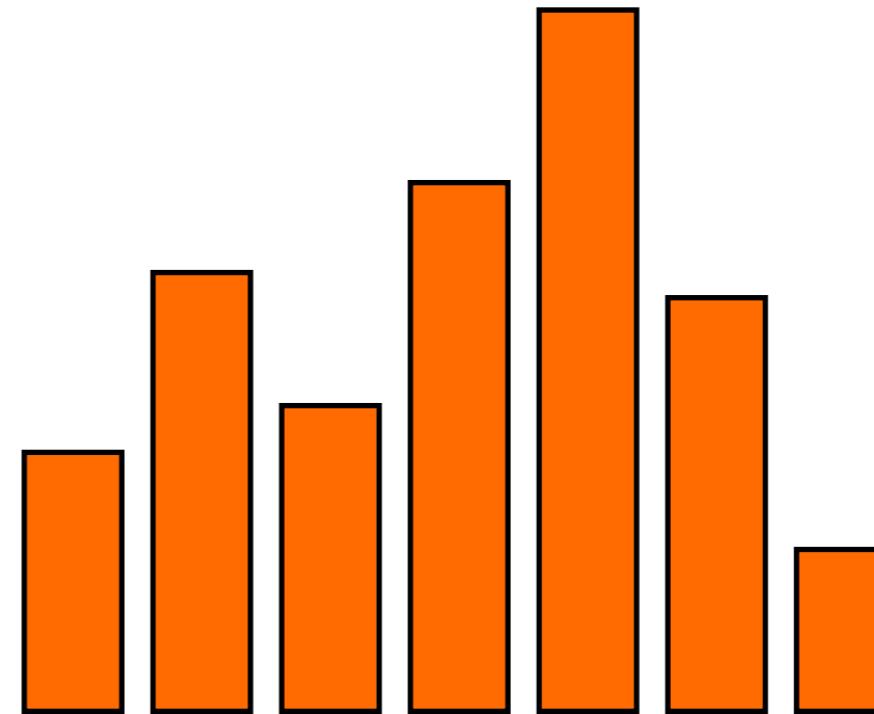
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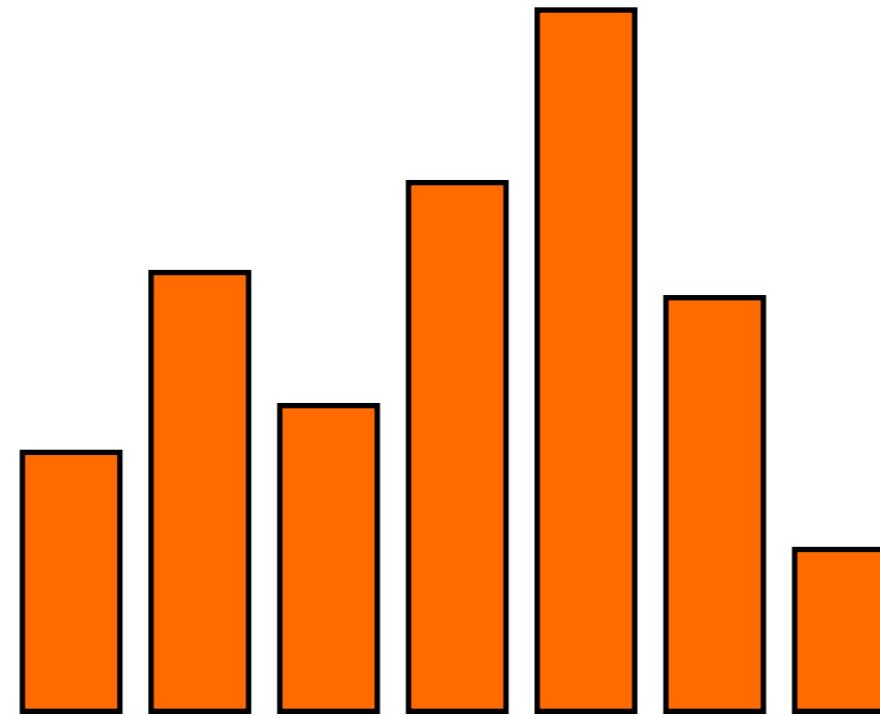
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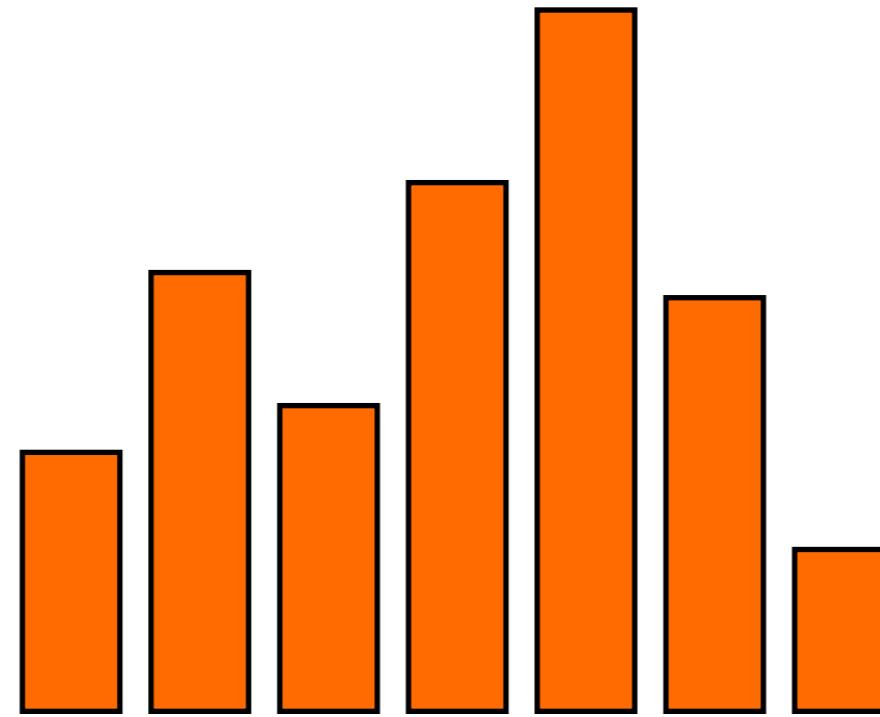
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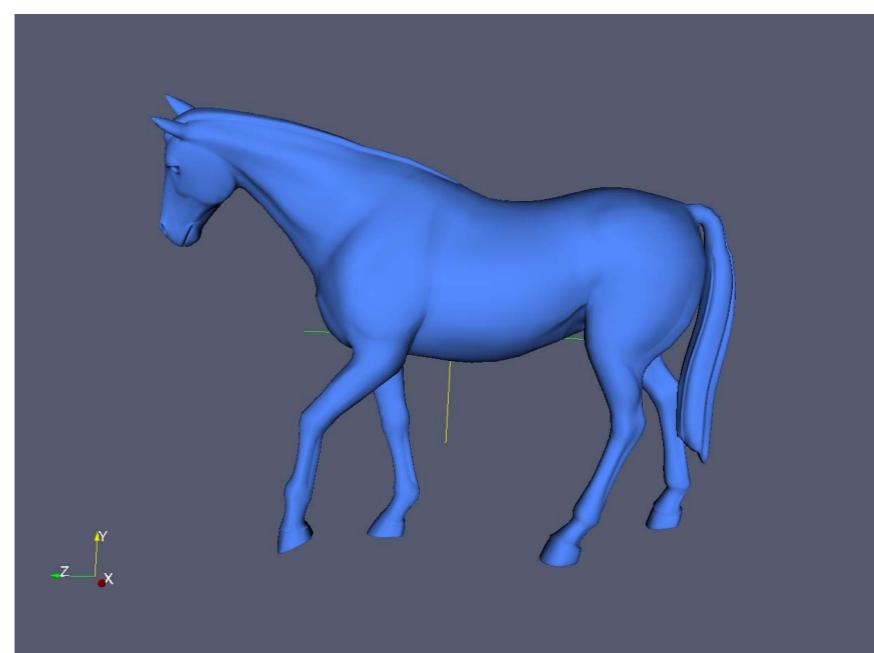
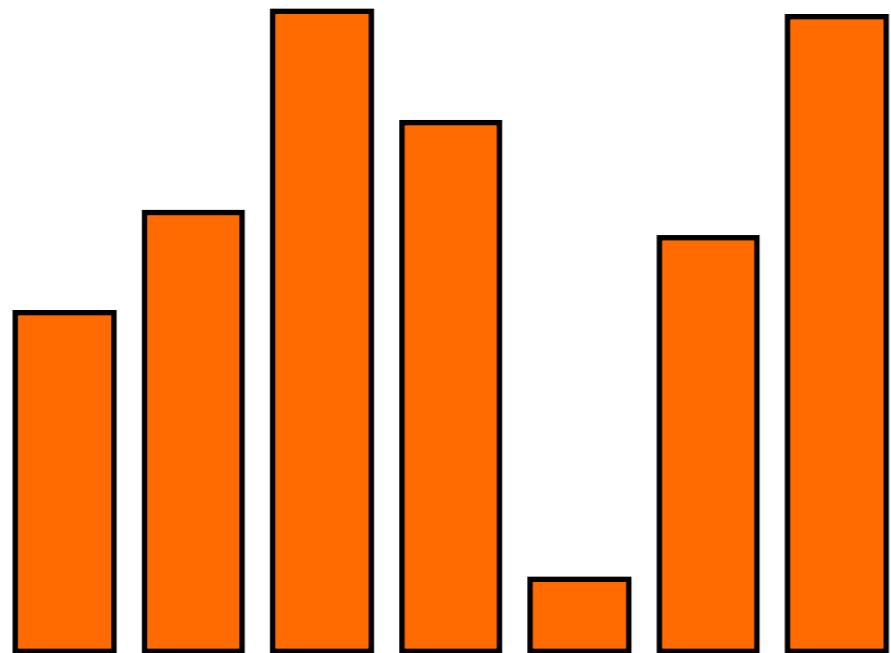
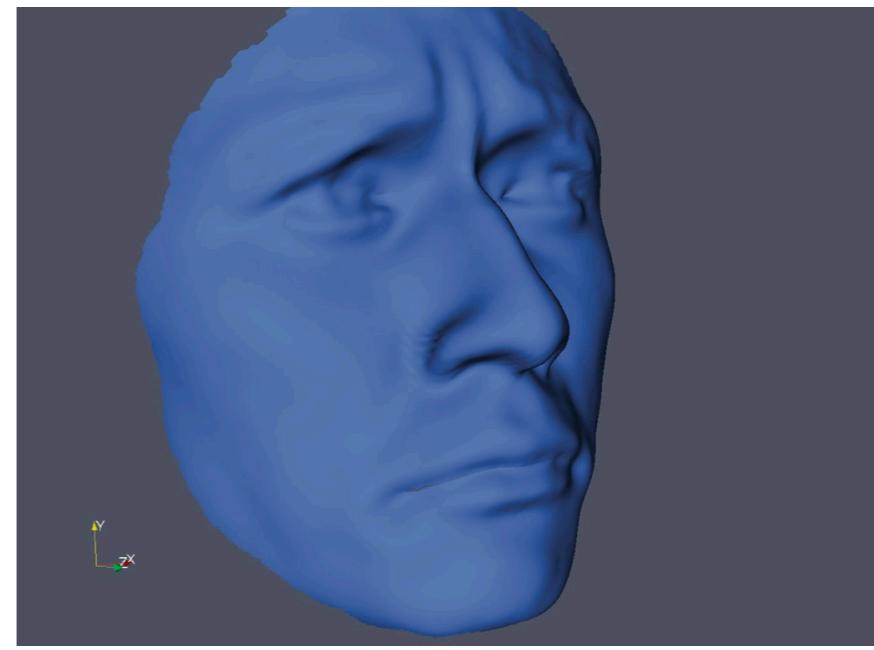
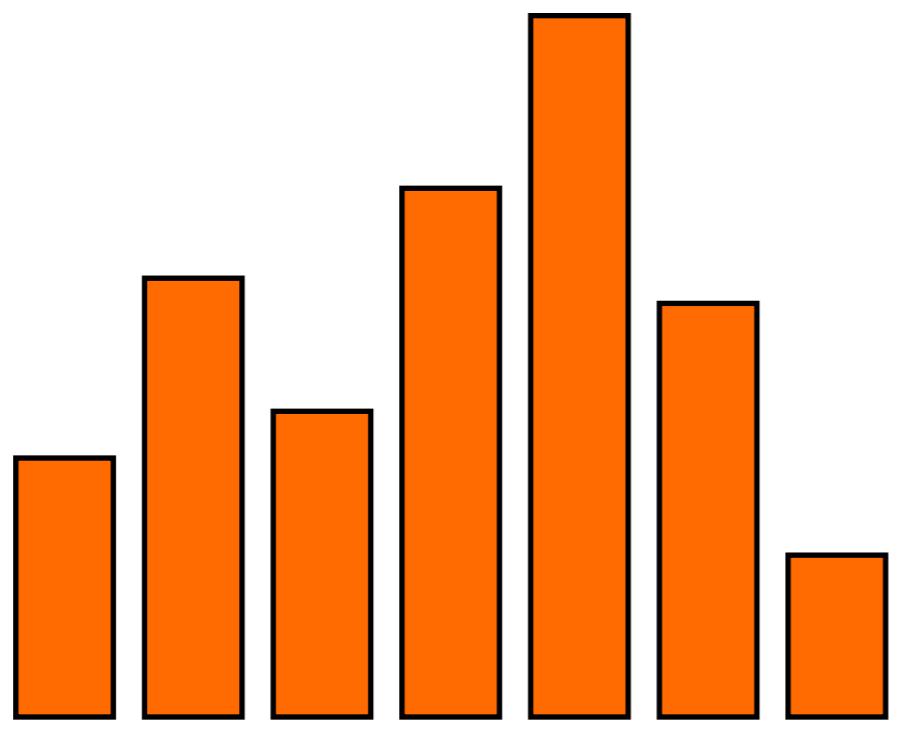
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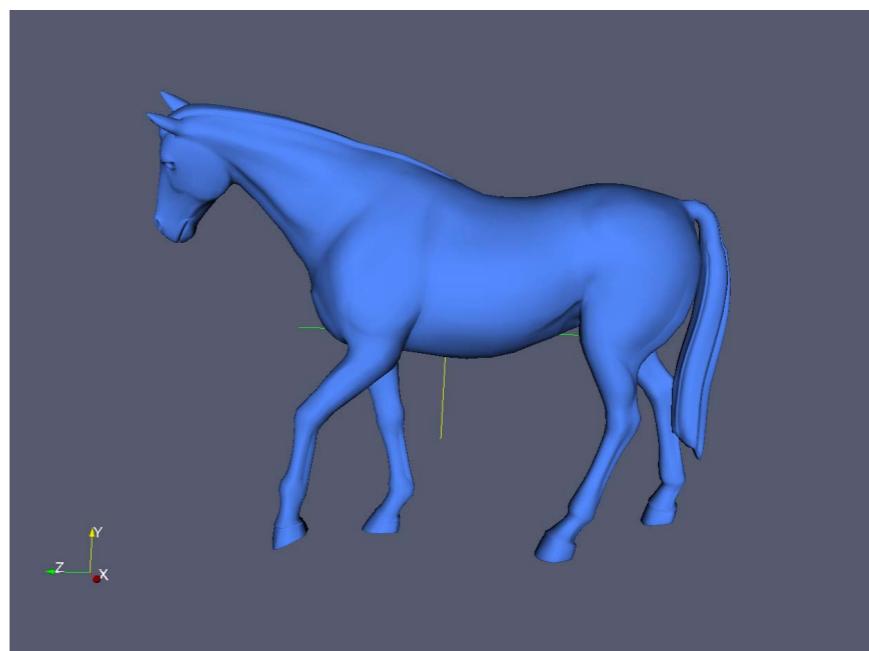
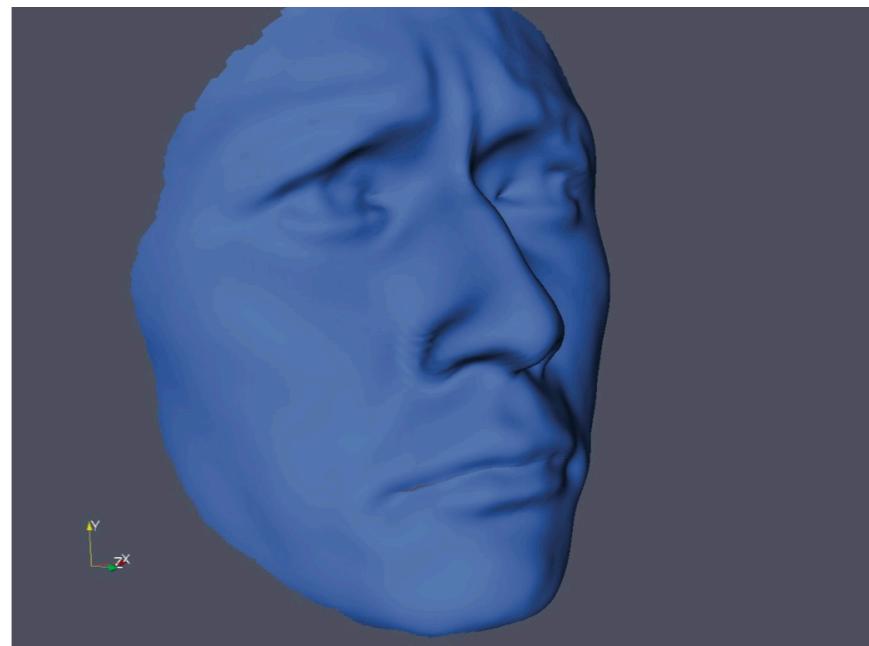
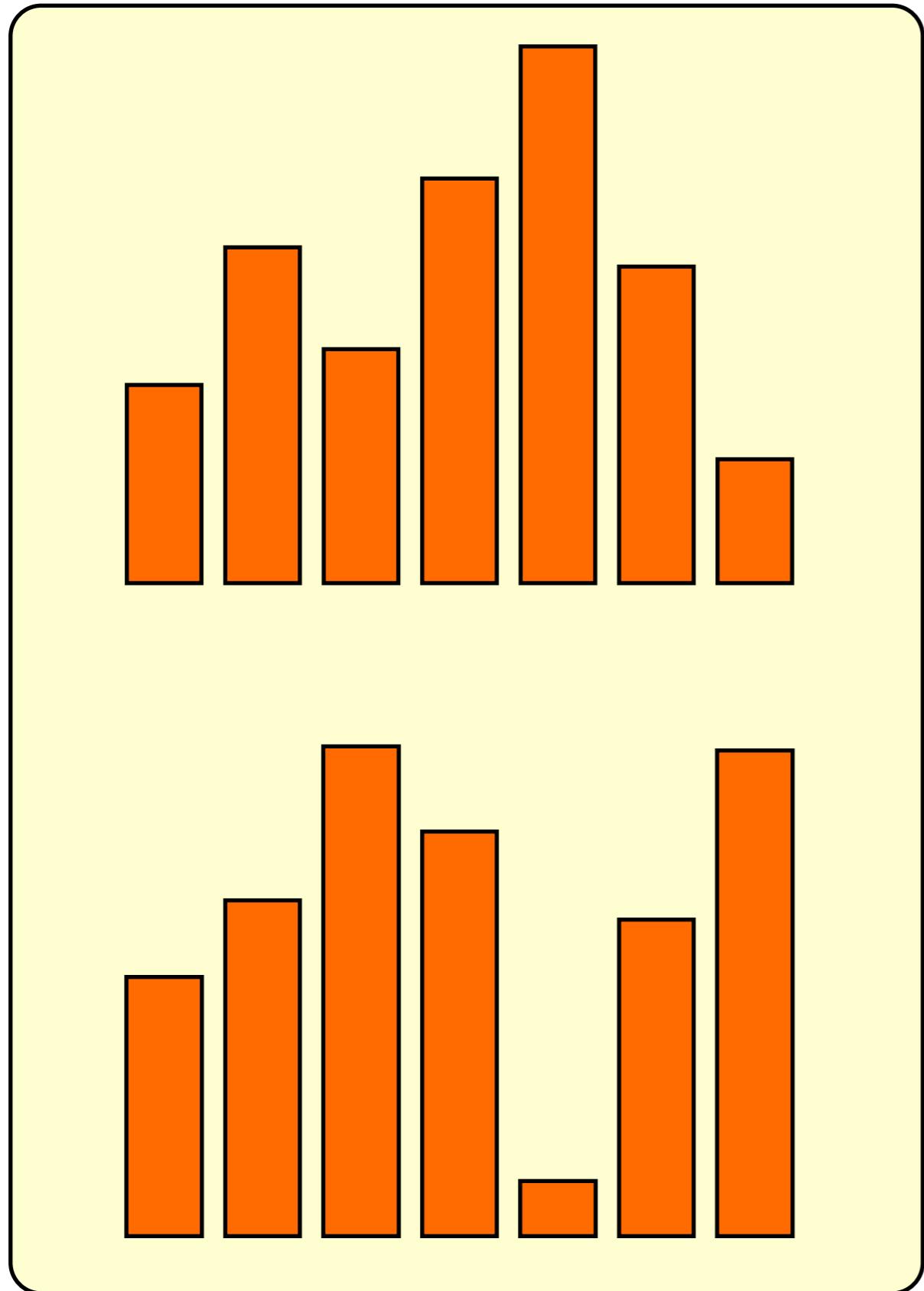


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Upper and Lower bounds Let (X, d, ν) be an mm-space.

- **Shape Distributions** [Osada-et-al]: construct histogram of interpoint distances, $F_X : \mathbb{R} \rightarrow [0, 1]$ given by

$$t \mapsto \nu \otimes \nu (\{(x, x') | d(x, x') \leq t\})$$

- **Shape Contexts** [SC]: at each $x \in X$, construct histogram of $d(x, \cdot)$, $C_X : X \times \mathbb{R} \rightarrow [0, 1]$ given by

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- **Hamza-Krim** [HK]: at each $x \in X$ compute mean distance to rest of points, $H_X : X \rightarrow \mathbb{R}$

$$x \mapsto \left(\int_X d^p(x, x') \nu(dx') \right)^{1/p}$$

- **Wasserstein under Euclidean isometries**: consider $X, Y \subset \mathbb{R}^d$ and compute

$$d_{\mathcal{W}, p}^{iso}(X, Y) = \inf_T d_{\mathcal{W}, p}(X, T(Y))$$

- **Gromov-Hausdorff distance** [MS04][MS05][BBK06]

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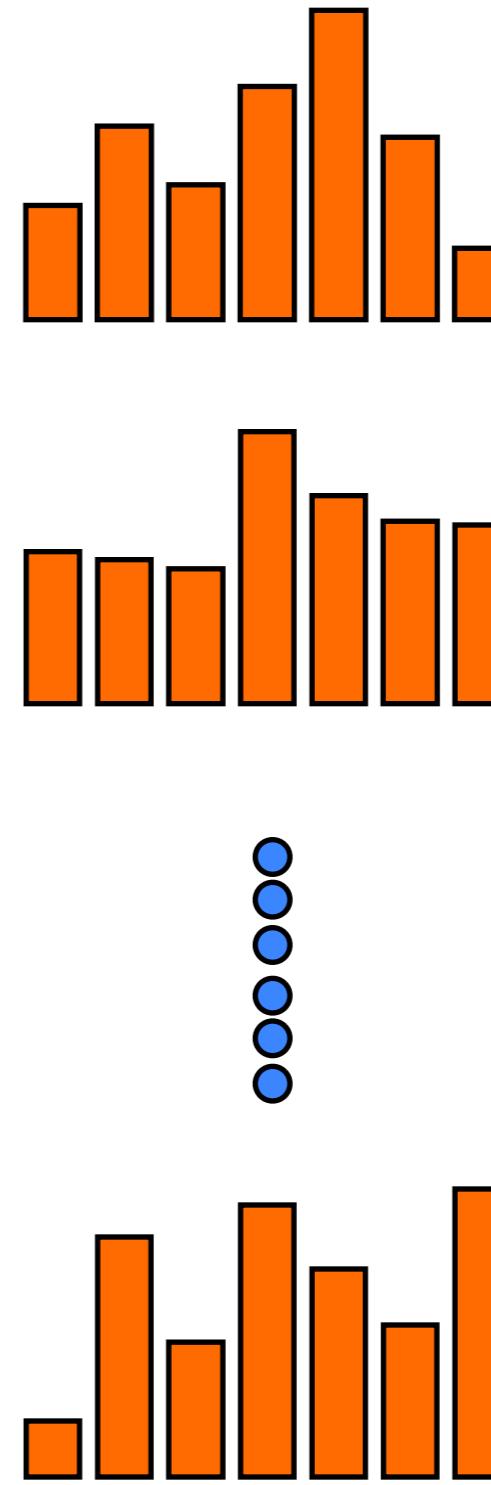
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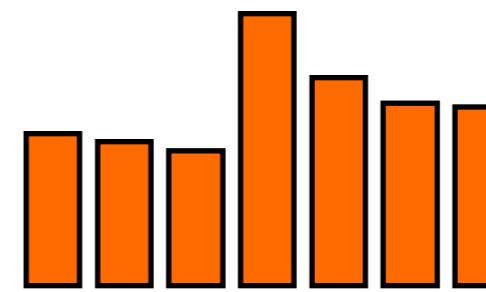
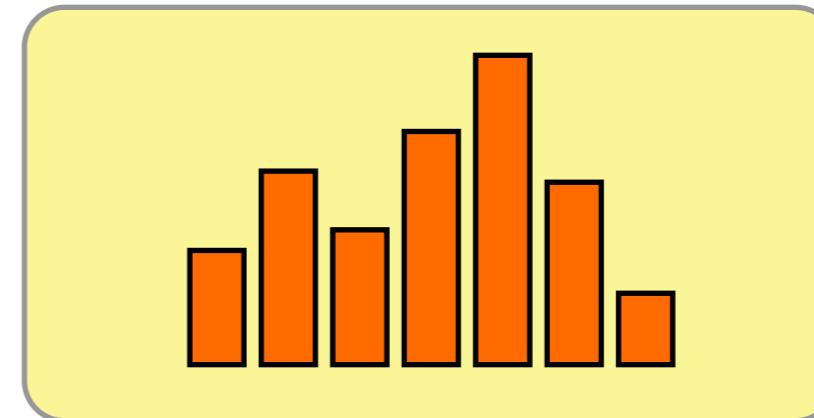
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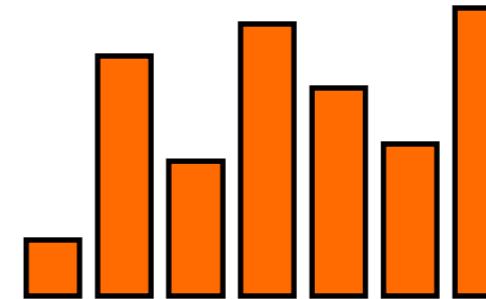


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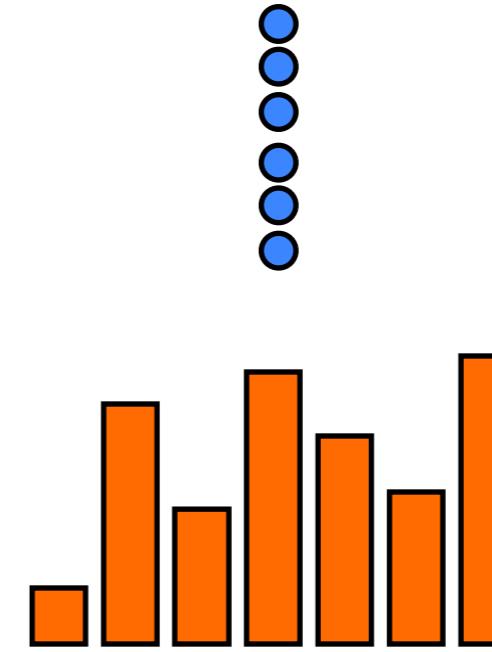
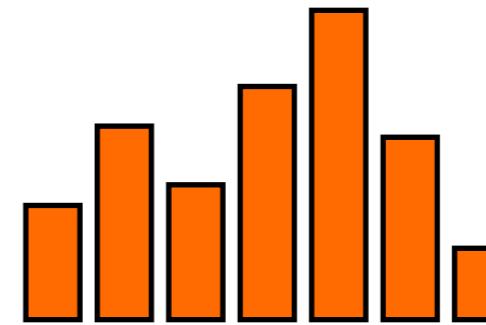
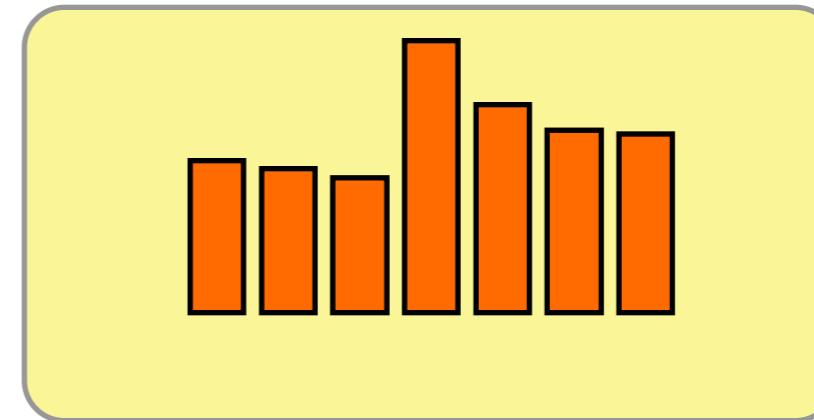


⋮



Shape Contexts

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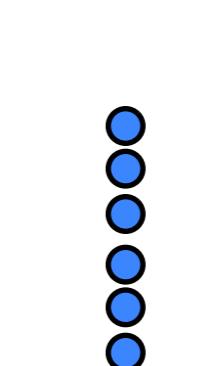
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The bound for the H-K approach

Let $p = 1$ for simplicity. For a mm-space (X, d_X, μ_X) let $s_X : X \rightarrow \mathbb{R}^+$ be given by

$$x \mapsto \sum_{x' \in X} \mu_X(x') d_X(x, x')$$

(average distance to all other points).

The HK lower bound, denoted by $LB_{HK}(X, Y)$ is defined to be (the mass transportation problem)

$$LB_{HK}(X, Y) := \min_{\mu \in \mathcal{M}(\mu_X, \mu_Y)} \sum_{x, y} \mu(x, y) |s_X(x) - s_Y(y)|.$$

Proposition 1 ([M07]). *For all mm-spaces X and Y ,*

$$\frac{1}{2} LB_{HK}(X, Y) \leq \mathbf{D}_1(X, Y)$$

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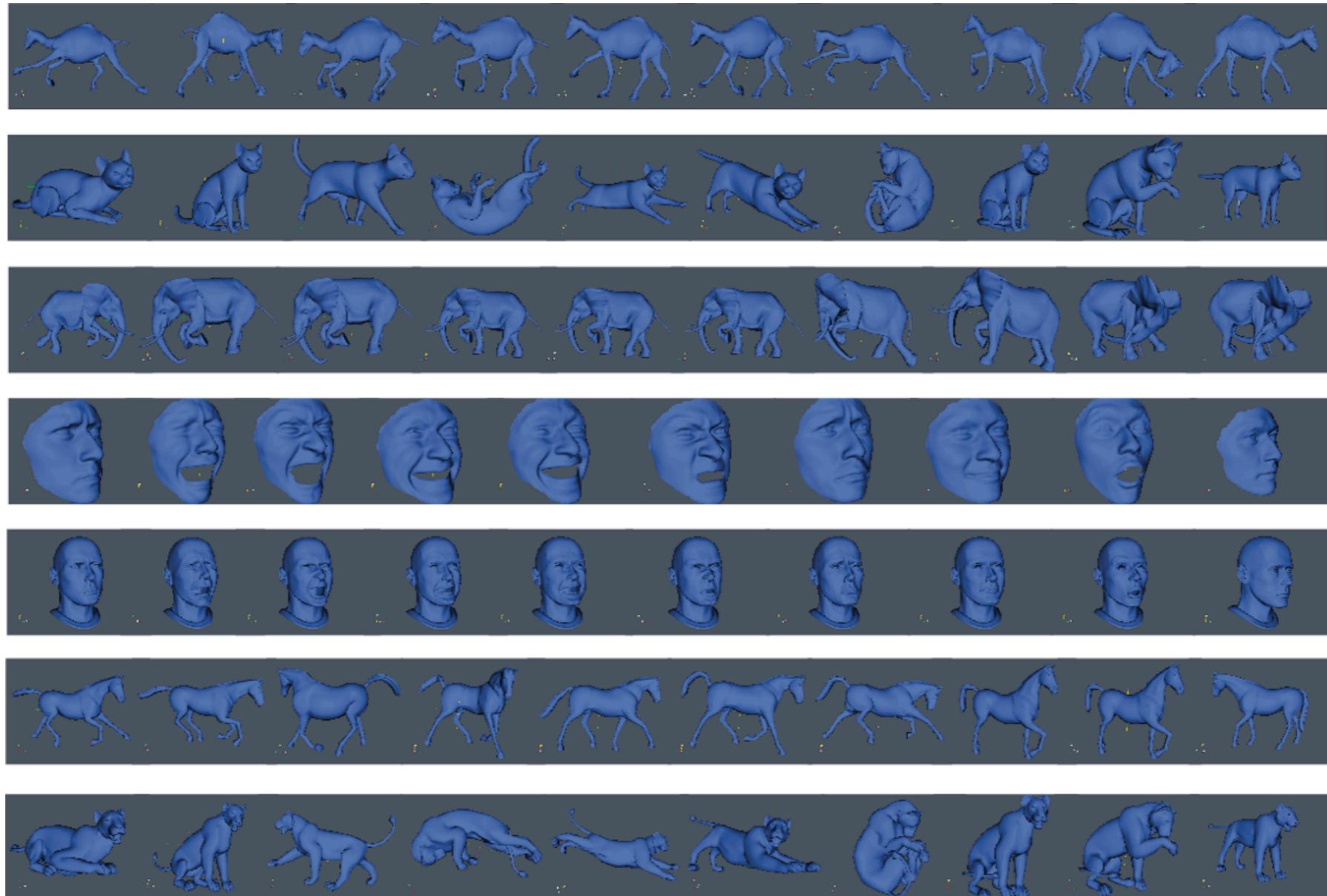
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Proof. Take any $\mu \in \mathcal{M}(\mu_X, \mu_Y)$ and write

$$\begin{aligned}
& \sum_{x,y} \sum_{x',y'} |d_X(x, x') - d_Y(y, y')| \mu(x, y) \mu(x', y') = \\
& \sum_{x,y} \sum_{x',y'} |\mu(x', y') (d_X(x, x') - d_Y(y, y'))| \mu(x, y) \geq \\
& \sum_{x,y} \underbrace{\left| \sum_{x',y'} \mu(x', y') (d_X(x, x') - d_Y(y, y')) \right|}_{\left\{ \sum_{x',y'} \mu(x', y') d_X(x, x') = \sum_{x'} d_X(x, x') \sum_{y'} \mu(x', y') = \sum_{x'} \mu_X(x') d_X(x, x') = s_X(x) \right\}} \mu(x, y) = \\
& \sum_{x,y} |s_X(x) - s_Y(y)| \mu(x, y) \geq \\
& LB_{HK}(X, Y)
\end{aligned}$$

The last inequality follows since μ was arbitrary and LB_{HK} was defined as the minimum.
To finish the proof, take the min over all choices of μ in $\mathcal{M}(\mu_X, \mu_Y)$ and recall definition of \mathbf{D}_1 .

Some Experiments



Some experimentation: ~ 70 models in 7 classes. Classification using 1-nn:
 $P_e \sim 2\%$. Hamza-Krim gave $\sim 15\%$ on same db with all same parameters etc.

Discussion

*Identifying a notion of **distance/metric** between shapes is useful/important.*

- When will you say that two shapes are the same? This is the zero of your distance between shapes.
- Having a true metric on the space of shapes permits proving *stability* and having a *sampling theory*.
- Understand hierarchy of lower/upper bounds. When is a particular LB better than another? study highly symmetrical shapes.

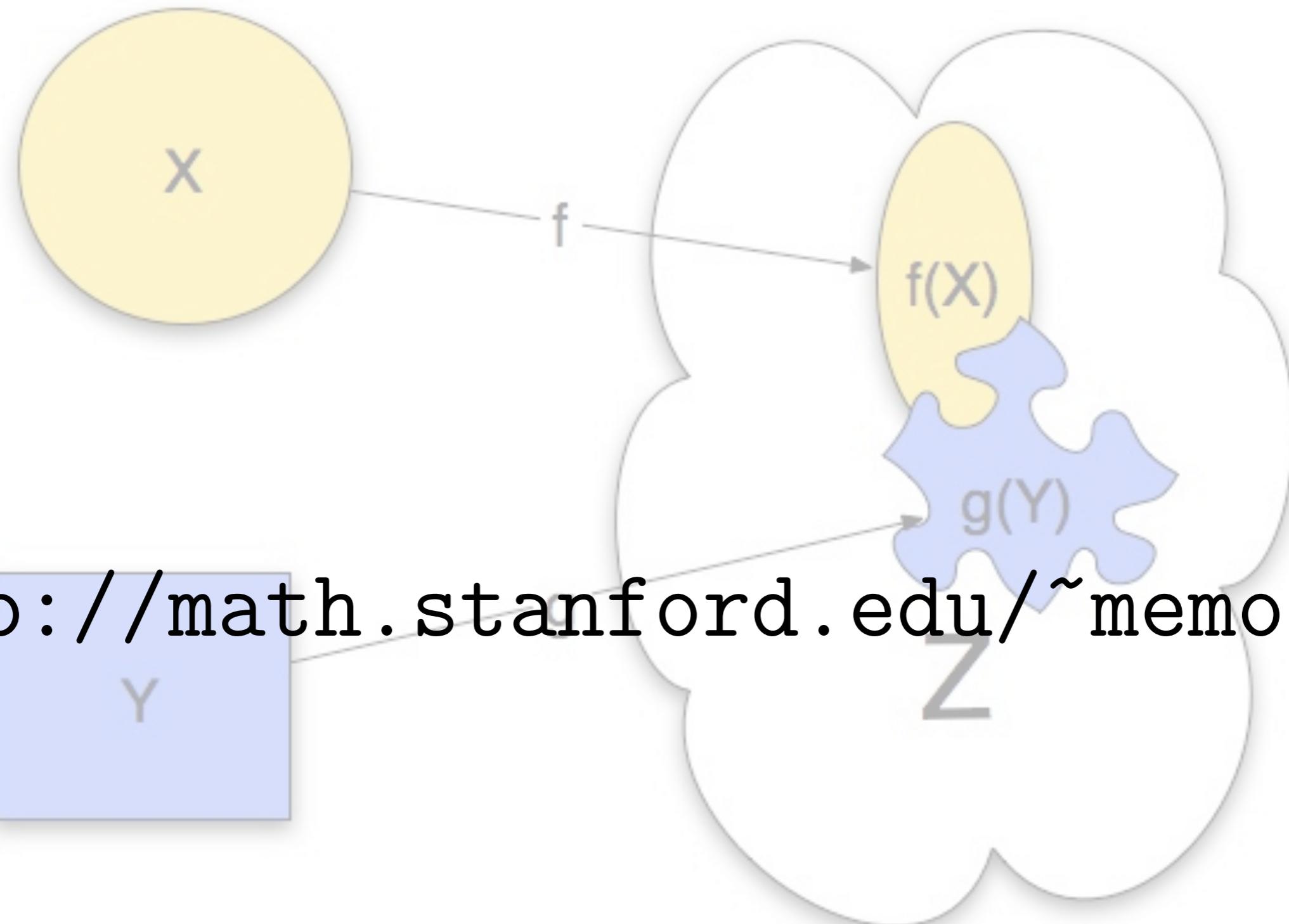
Discussion

- Implementation is easy: Gradient descent or alternate opt.
- Solving lower bounds yields a seed for the gradient descent. These lower bounds are compatible with the metric in the sense that a layered recognition system is possible: given two shapes, (1) solve for a LB (this gives you a μ), if value small enough, then (2) solve for GW using the μ as seed for your favorite iterative algorithm.
- Easy extension to **partial matching**— preprint available from my webpage soon.
- Interest in relating GH/GW ideas to other methods in the literature. Interrelating methods is important also for applications: when confronted with N methods, how do they compare to each other? which one is better for the situation at hand?
 - Euclidean case.
 - Persistent Topology based methods (Frosini et al., Carlsson et al.)
- No difference between continuous and discrete. Probability measures take care of the 'transition'.

<http://math.stanford.edu/~memoli/ShapeComp/sc.html>

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