

Shape Matching and Metric Geometry

Facundo Mémoli.

CS 5339, The Ohio State University, Spring 2014.

Shape Matching and Metric Geometry

Course Info

Instructor [Facundo Mémoli](#), memoli@math.osu.edu

Course code CSE 5339 -- Spring 2014

Times: Mondays 3-4:50 PM.

Location: **BE 184.** [Map](#)

Description: This course will touch upon the use of ideas from metric geometry for tackling the problem of Matching/Comparison of Shapes under invariances.

The central idea is to consider shapes as metric spaces (or measure metric spaces) and, then, use one of various notions of distance between metric spaces to obtain a measure of dissimilarity between shapes. Connections with several standard approaches to the problem of shape comparison will be discussed.

The choice of the metric with which one augments the shapes encodes the degree of invariance one obtains from the dissimilarity measure. The main example in this family of notions of dissimilarity between shapes is the Gromov-Hausdorff distance.

We will start by reviewing the main approaches in the literature. Then we will discuss the requisite theoretical background from Metric Geometry and cover details about the numerical computation of lower bounds to the Gromov-Hausdorff distances.

Several possible research directions will be discussed.

Prerequisites: The course has minimal requisites: it is designed for students from Computer Science and Engineering, and Mathematics having knowledge of undergrad level math. Some knowledge of geometry will be useful, but not necessary. The course will provide the opportunity to explore different aspects of the material: interested students will have the opportunity of implementing some algorithms and/or exploring some research papers on different aspects of both the underlying mathematics and/or the algorithmic procedures.

General stuff:

- class attendance is mandatory
- will post possible papers soon, after we discuss some more.
- 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.
 - [**dGW**] my 2011 FoCM paper.
 - [**M07**] my PBG07 paper.
 - etc

Grading

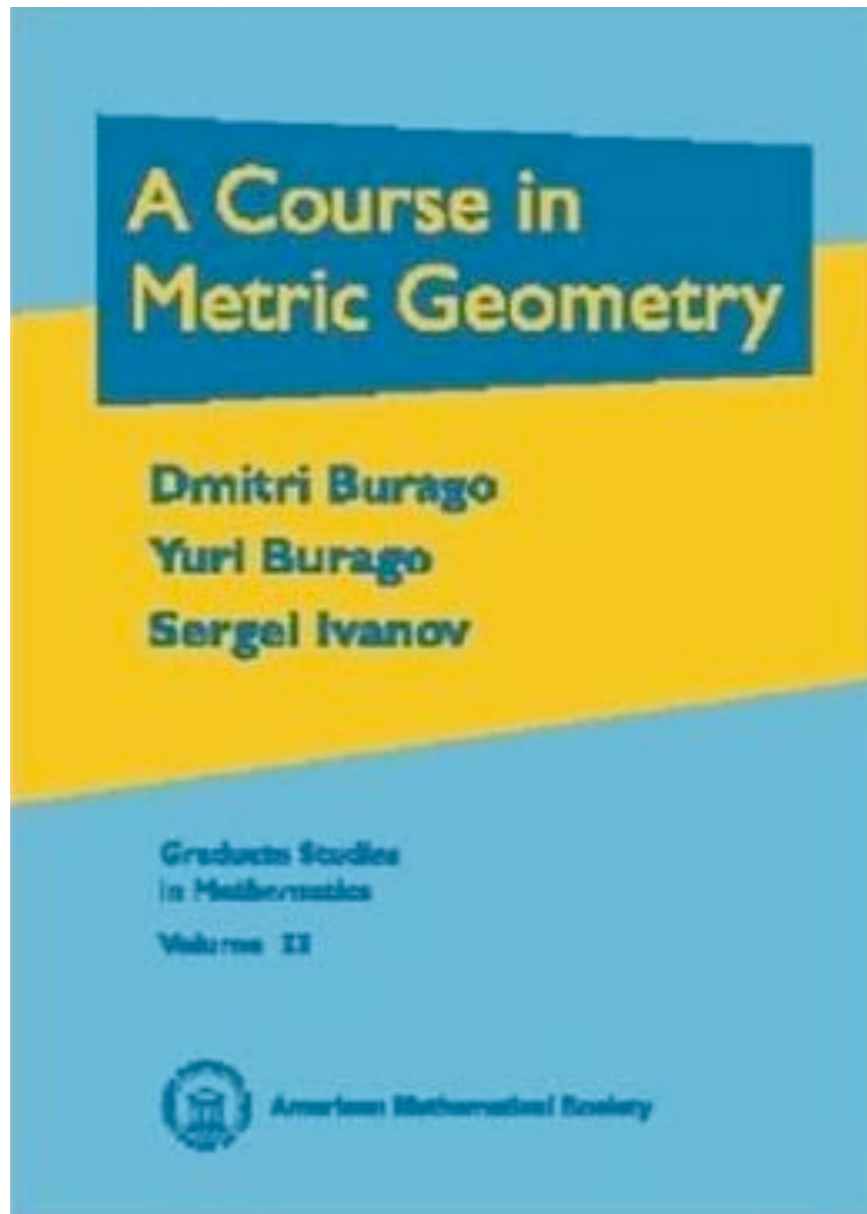
The grade will be based on three components. Everyone will be involved in (1) presenting paper(s) and in (2) a final project. The project will be based on reading a number of papers and then presenting them in class and writing up a report. Topics and emphasis will depend on the interest of each student. Some projects may be about studying and implementing some algorithms, while others could revolve around studying a set of more theoretical ideas. There will be no exam.

- **Paper presentation:** 35%. Some of the classes will be seminar style where we will take turns presenting and discussing papers.
- **Final project:** 50%. This includes both the talk (25%) and the report (25%).
- **Class participation:** 15%. This includes a number of reading assignments.

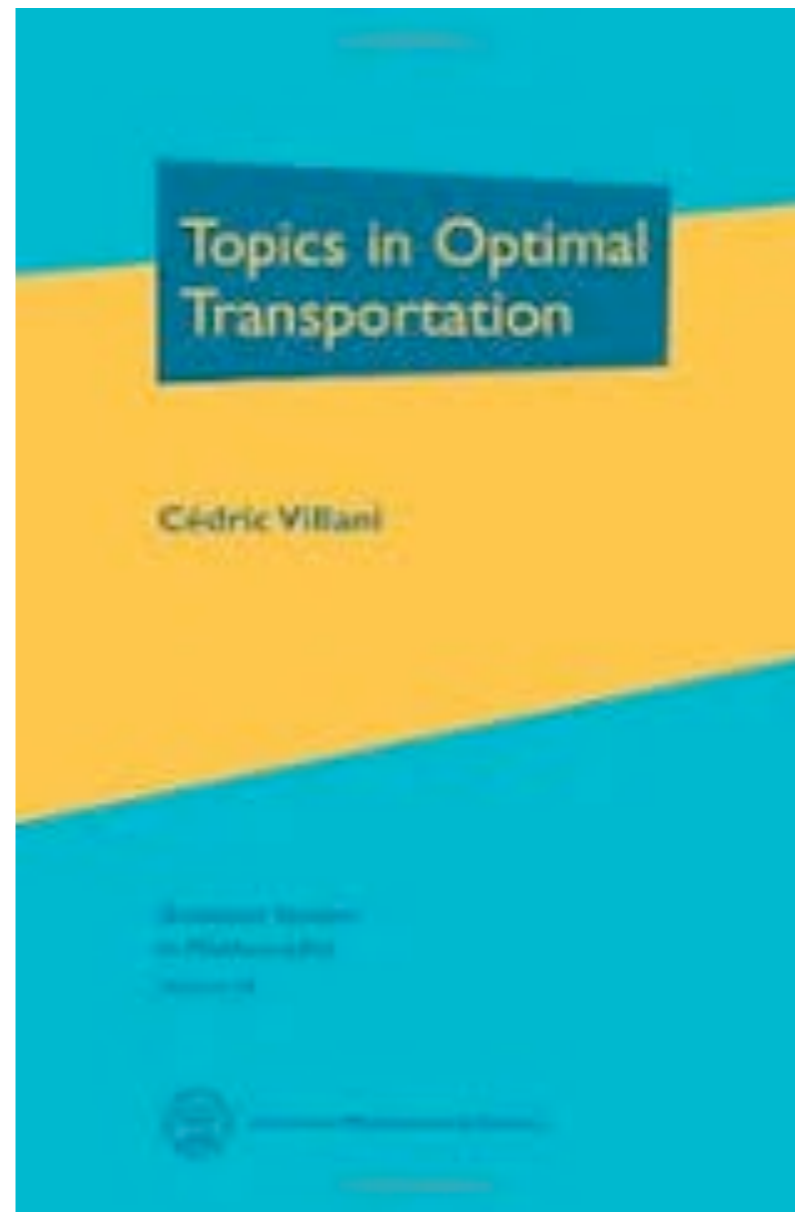
office hours etc

send me an email and we'll set up a meeting.

a couple of reference books:



[BBI]



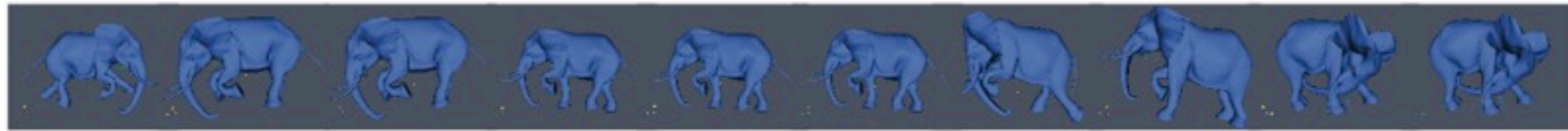
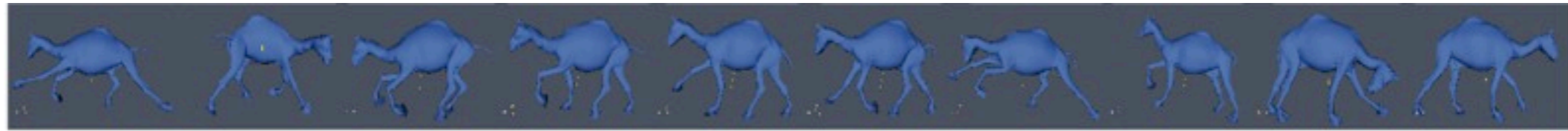
[Villani]

Note: these are **not** textbooks

**introduction/motivation: shape matching, shape
comparison, shape analysis**

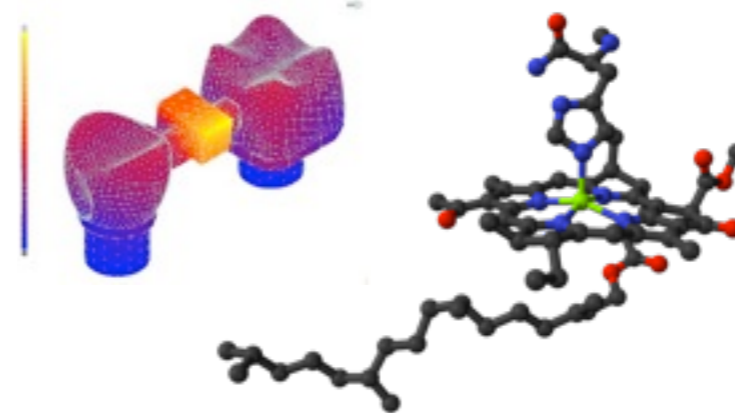
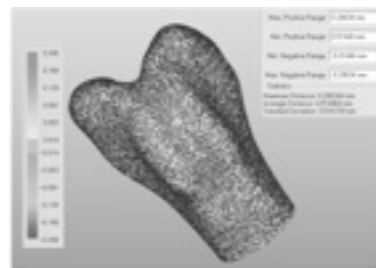
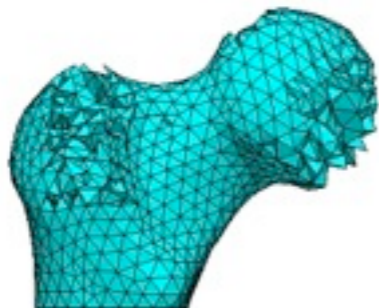
The Problem of Shape/Object Matching

- 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 prostheses
 - 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>





- 3D scanners are becoming increasingly cheaper.
- consequence: lots of 3D data are being generated and stored.
- 3D printing!
- How do we organize those datasets?

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Ads related to 3d scanners









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<http://sketchup.google.com/3dwarehouse/>

3D Modeling Pipeline for Google Earth is now retired. [Read more](#)

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[Herman Miller Aeron Chair \(Dynamic\)](#)
by [SmartFurniture.com](#)

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Michelangelo

Sculptor

Michelangelo di Lodovico Buonarroti Simoni, commonly known as Michelangelo, was an Italian sculptor, painter, architect, poet, and engineer of the High Renaissance who exerted an unparalleled influence on the development of Western art. [Wikipedia](#)

Born: March 6, 1475, [Caprese Michelangelo, Italy](#)

Died: February 18, 1564, [Rome, Italy](#)

Buried: [Basilica of Santa Croce, Florence, Italy](#)

Structures: [St. Peter's Basilica](#), [Laurentian Library](#), [More](#)

Periods: Italian Renaissance, High Renaissance, Renaissance





Our project logo
(click here to read about its [design](#))

The Digital Michelangelo Project



Our laser scan of the David
(click here for [more images](#))

 [Versione Italiana](#)

News flashes:

- 7/21/09 - We now have a full-resolution (1/4mm) [3D model](#) of Michelangelo's 5-meter statue of David. The model contains about 1 billion polygons.
- 8/03/04 - A [SIGGRAPH 2004 paper](#) describing the technology underlying our [ScanView](#) system.
- 5/29/04 - Check out two new photographic essays, about a [physical replica](#) of the David, and on a [new book](#) about restoring the statue.
- 8/27/03 - Download [ScanView](#): a program that lets you fly around our models of Michelangelo's statues - no license required.

About the project

Introduction

Recent improvements in laser rangefinder technology, together with algorithms developed at Stanford for combining multiple range and color images, allow us to reliably and accurately digitize the external shape and surface characteristics of many physical objects. Examples include machine parts, cultural artifacts, and design models for the manufacturing, moviemaking, and video game industries.

As an application of this technology, a team of 30 faculty, staff, and students from Stanford University and the University of Washington spent the 1998-99 academic year in Italy scanning the sculptures and architecture of Michelangelo. As a side project, we also scanned 1,163 fragments of the Forma Urbis Romae, a

CyArk 500 CHALLENGE

LAUNCH AND CONFERENCE
OCTOBER 20 - 22, 2013 / TOWER OF LONDON.

CyArk 500 Challenge Launch and Conference Website

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CyArk's
Mission

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Rome's Colosseum to be Restored

2 days ago

The Colosseum in Rome will be restored to remove a coating of "black rust" from traffic exhaust.

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Articles and Blogs



Call for CyArk 500 Project Submissions

December 17th, 2013

The first deadline for submissions is December 31!

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Featured Content



Tambo Colorado: Inca Center in Peru

2 days ago

Learn about this strategic Inca center which once dominated access to the main Inca road to the highlands and capital....

CyArk

From Wikipedia, the free encyclopedia

CyArk is a [501\(c\)\(3\)](#) nonprofit organization located in Oakland, California, United States. The company's website refers to it as a "digital archive of the world's heritage sites for preservation and education". Its official mission statement is "Digitally preserving cultural heritage sites through collecting, archiving and providing open access to data created by laser scanning, digital modeling, and other state-of-the-art technologies."

CyArk's founder, Ben Kacyra, stated during his speech at the 2011 [TED Conference](#) that the organization was created in response to increasing human and natural threats to heritage sites, and to ensure the "collective human memory" is not lost while making it available through modern dissemination tools like the internet and mobile platforms.

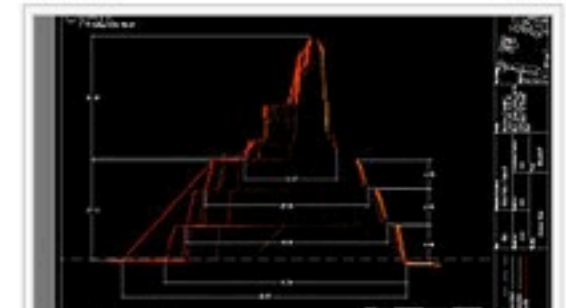


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History [\[edit\]](#)

CyArk was founded in 2003 by Iraqi expatriate and civil engineer Ben Kacyra. Kacyra was instrumental in the invention and marketing of the first truly portable [laser scanner](#) (called the [Cyrax](#)) designed for surveying purposes during the 1990s. After Kacyra's company (Cyra Technologies) and all rights to the invention were purchased by Swiss firm [Leica Geosystems](#) in 2001, Kacyra dedicated his energy to the application of the new technology to the documentation of archaeological and cultural heritage resources through CyArk. CyArk's primary focus has been the documentation and digital preservation of threatened ancient and historical architecture found at sites such as



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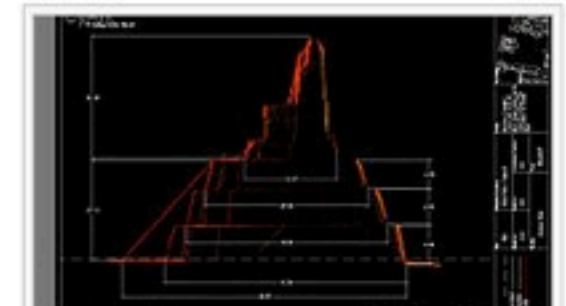


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TALKS

Ben Kacyra: Ancient wonders captured in 3D

FILMED JUL 2011 • POSTED NOV 2011 • TEDGlobal 2011



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Ancient monuments give us clues to astonishing past civilizations – but they're under threat from pollution, war, neglect. Ben Kacyra, who invented a groundbreaking 3D scanning system, is using his invention to scan and preserve the world's heritage in archival detail. (Watch to the end for a little demo.)

Ben Kacyra uses state-of-the-art technology to preserve cultural heritage sites and let us in on their secrets in a way never before possible. [Full bio »](#)

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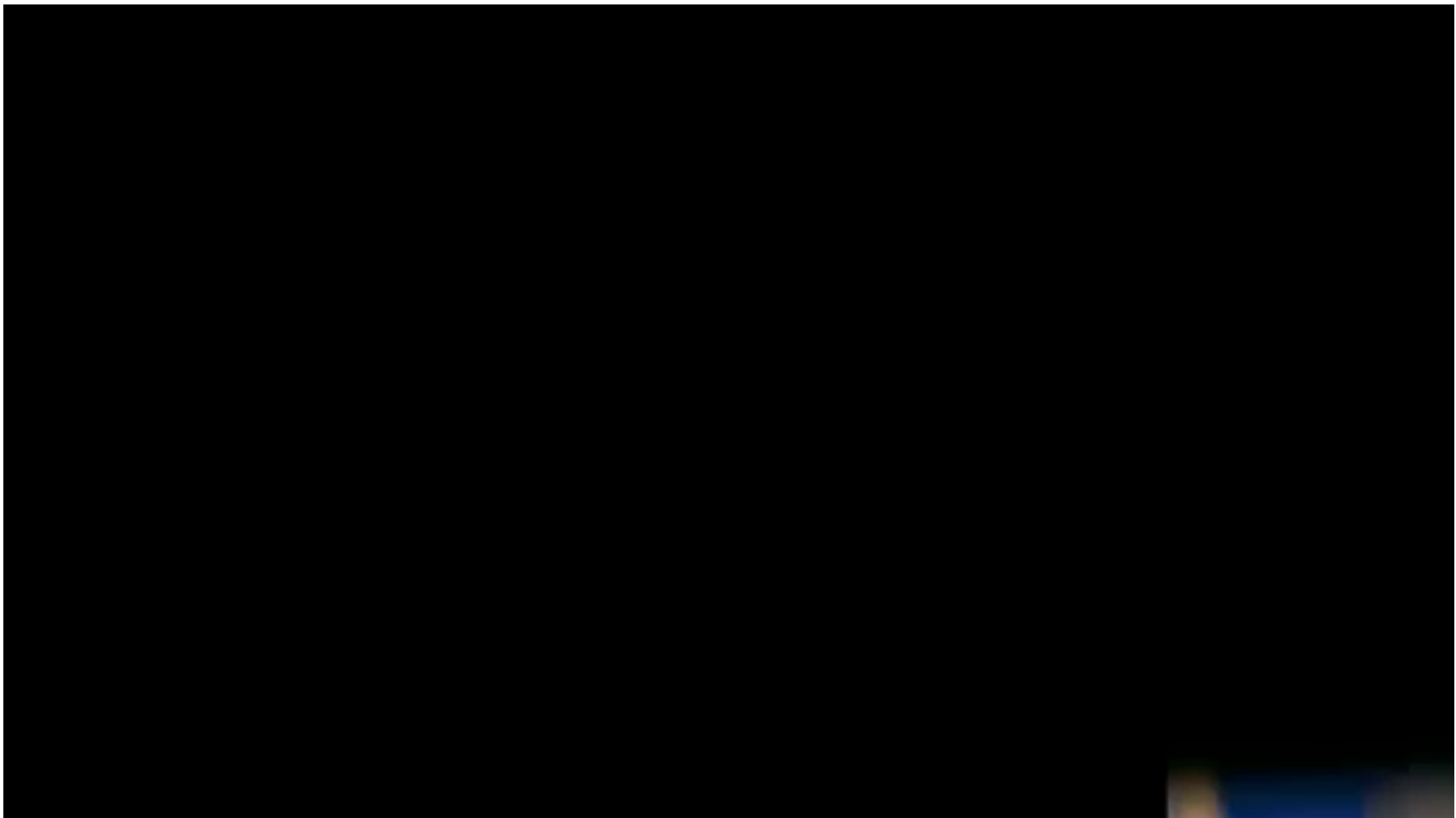


Where do ideas come from?

Curated by TED

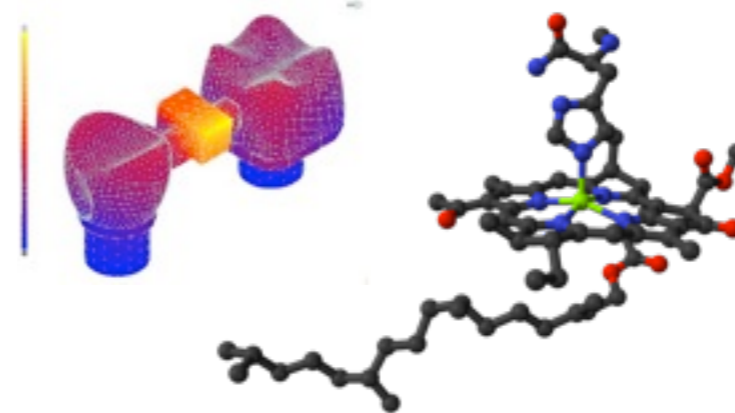
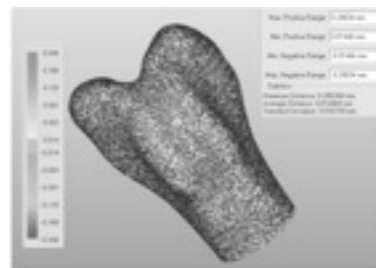
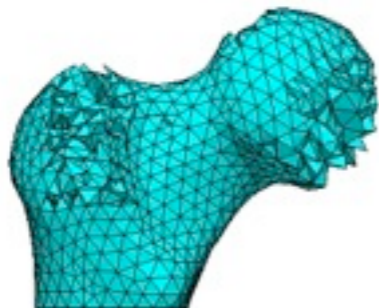
How does the metaphorical lightbulb go off? Is it a flash of genius? The power of crowds? These heady talks explore the nature of ideas...

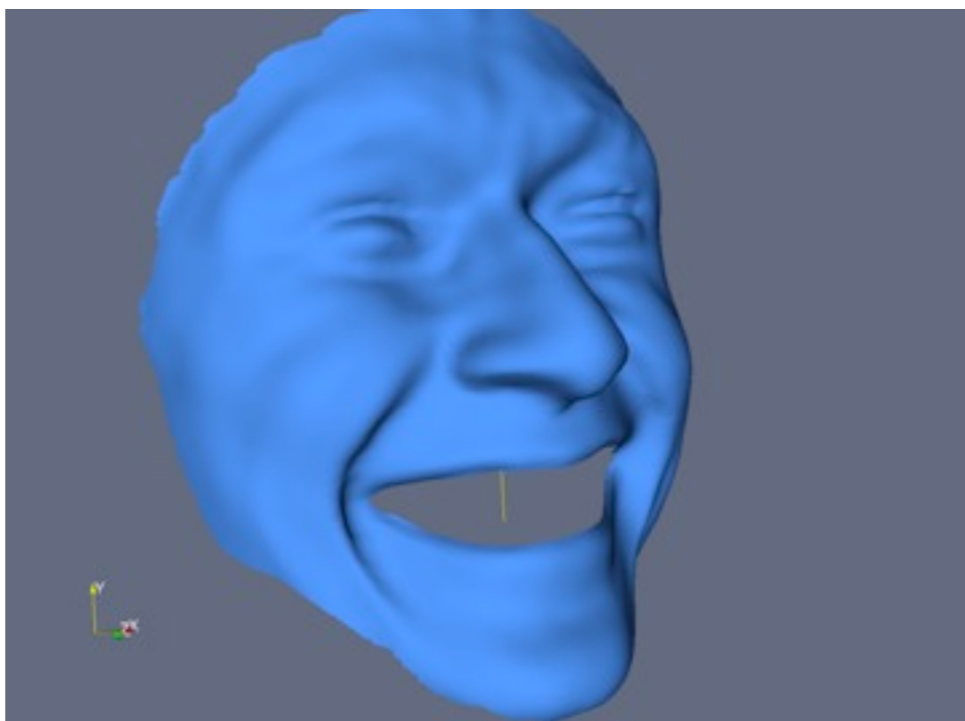
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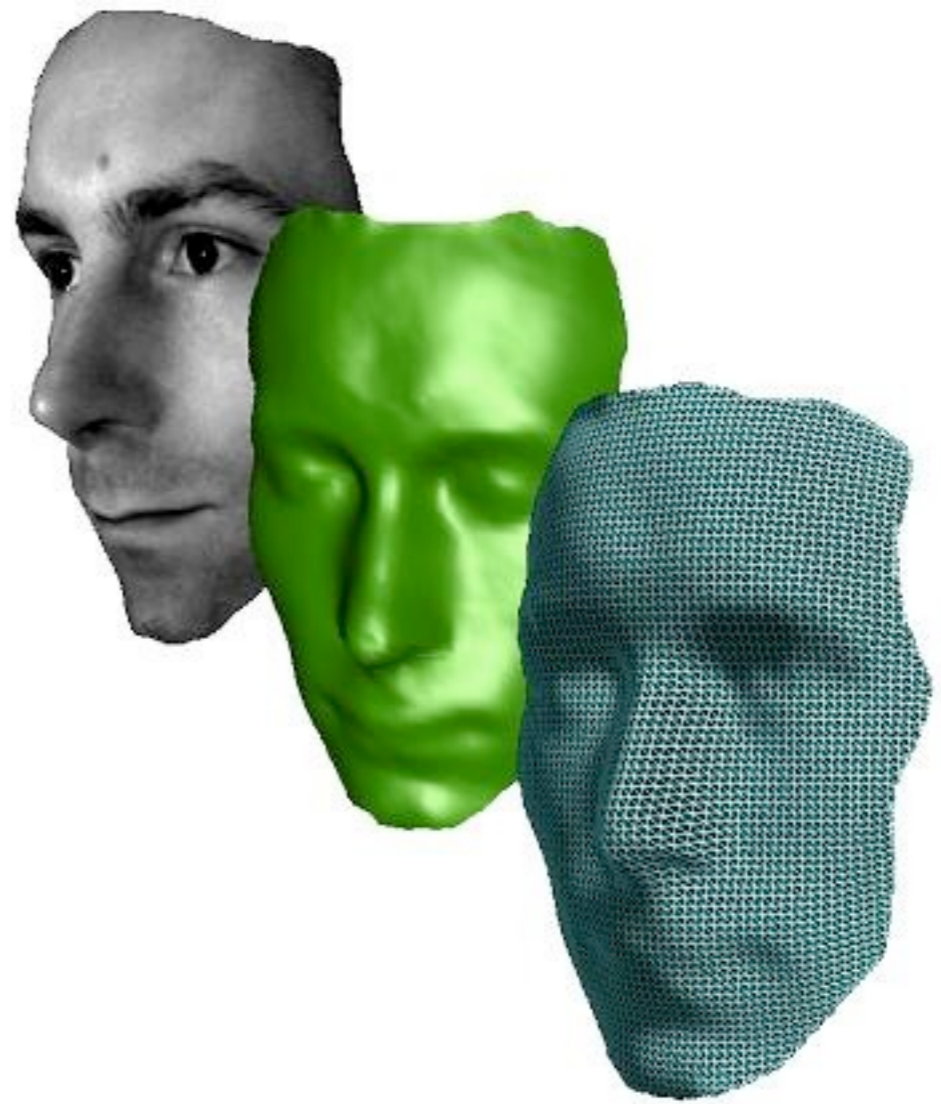


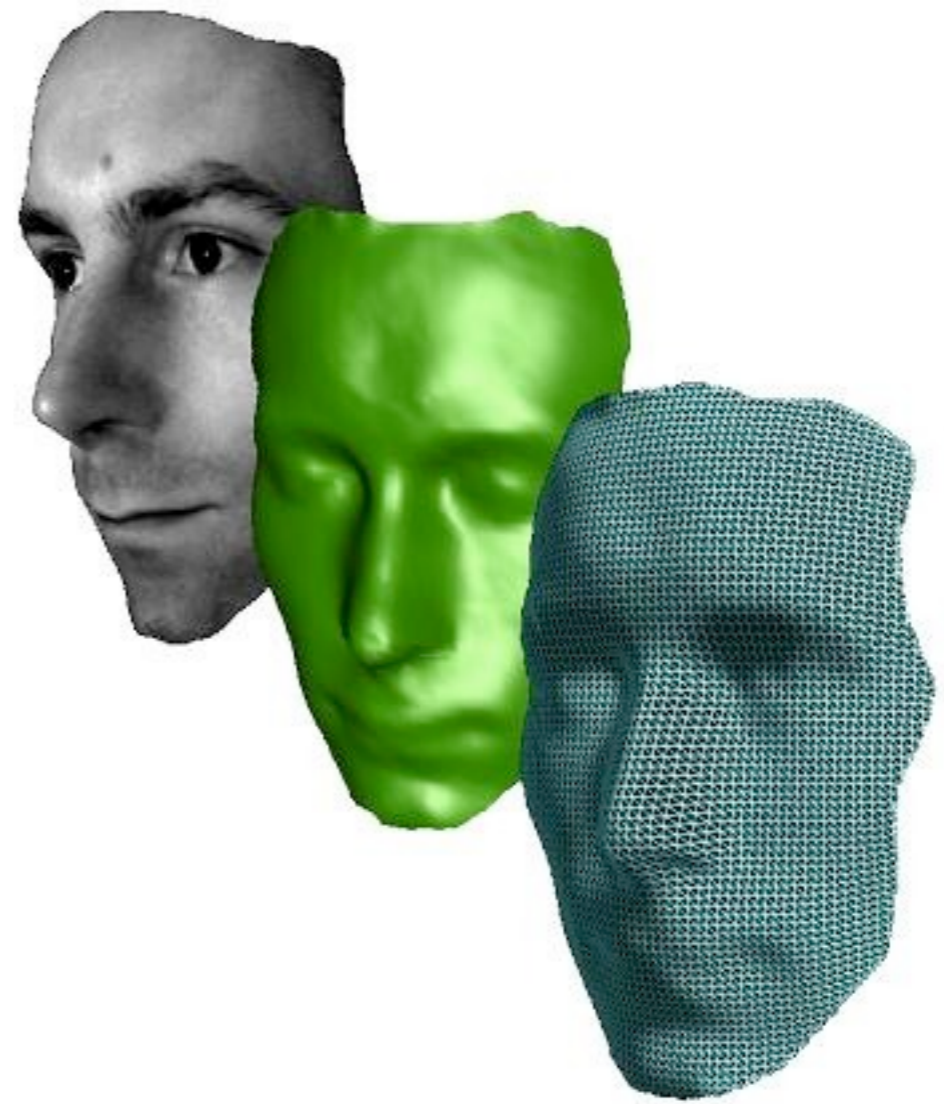
3D objects: examples

- 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>









3D Face Biometrics 2013

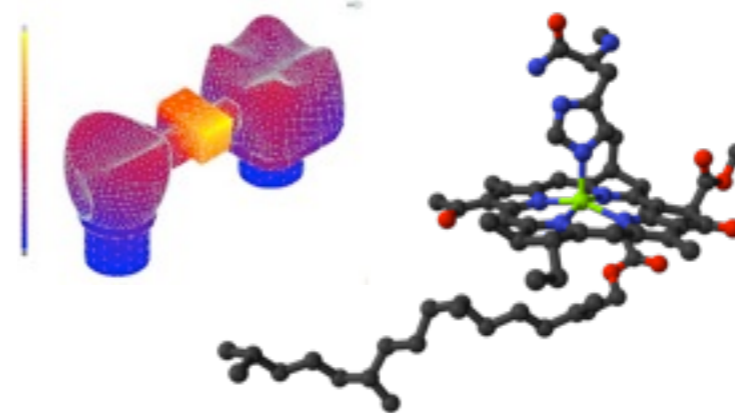
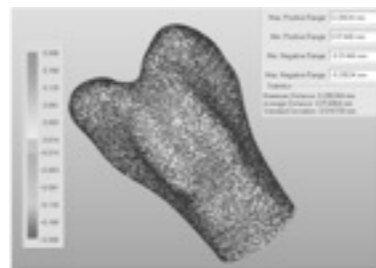
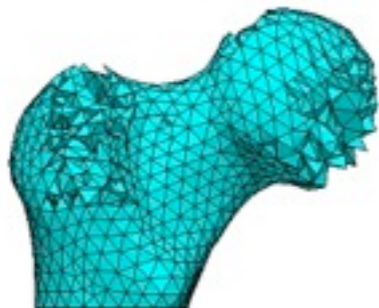
Shanghai, China - April 22, 2013

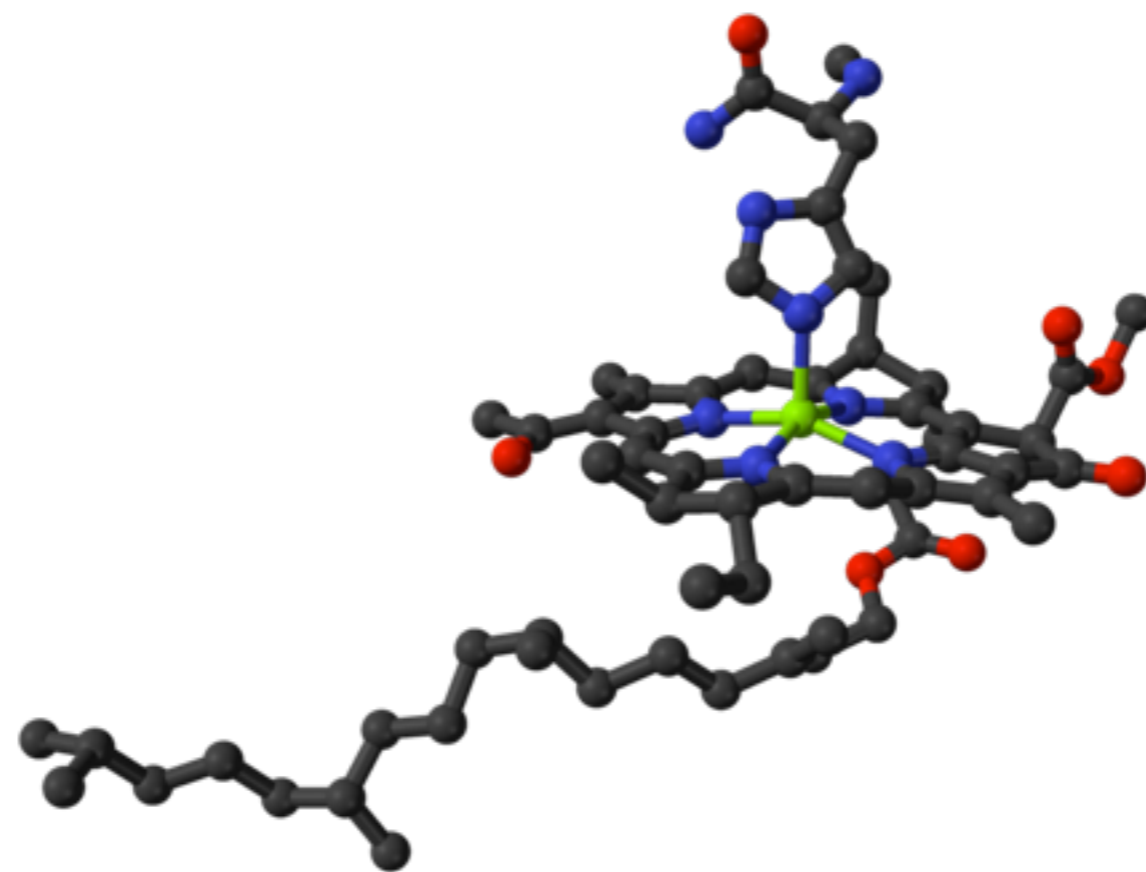
In conjunction with the 10th IEEE International Conference on Automatic Face and Gesture Recognition



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Structural biology

From Wikipedia, the free encyclopedia

Structural biology is a branch of [molecular biology](#), [biochemistry](#), and [biophysics](#) concerned with the molecular structure of biological [macromolecules](#), especially [proteins](#) and [nucleic acids](#), how they acquire the structures they have, and how alterations in their structures affect their function. This subject is of great interest to biologists because macromolecules carry out most of the functions of [cells](#), and because it is only by coiling into specific three-dimensional shapes that they are able to perform these functions. This architecture, the "[tertiary structure](#)" of molecules, depends in a complicated way on the molecules' basic composition, or "[primary structures](#)."

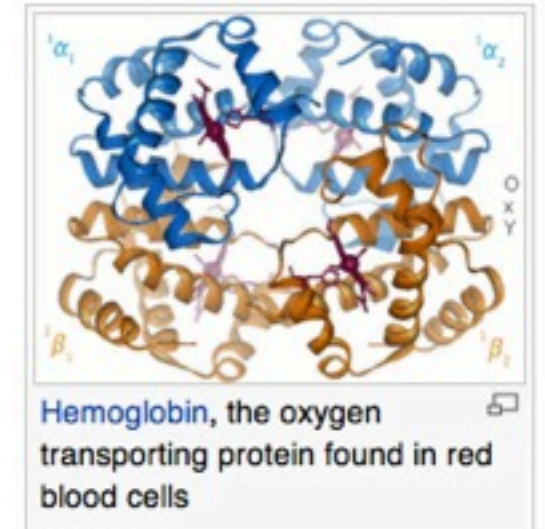
[Biomolecules](#) are too small to see in detail even with the most advanced light [microscopes](#). The methods that structural biologists use to determine their structures generally involve measurements on vast numbers of identical molecules at the same time. These methods include:

- [Macromolecular crystallography](#)
- [Proteolysis](#)
- [NMR](#)
- [EPR](#)
- [Cryo-electron microscopy \(cryo-EM\)](#)
- [Multiangle light scattering](#)
- [Small angle scattering](#)
- [Ultra fast laser spectroscopy](#)
- [Dual Polarisation Interferometry and circular dichroism](#)

Most often researchers use them to study the "[native states](#)" of macromolecules. But variations on these methods are also used to watch nascent or [denatured](#) molecules assume or reassume their native states. See [protein folding](#).

A third approach that structural biologists take to understanding structure is [bioinformatics](#) to look for patterns among the diverse [sequences](#) that give rise to particular shapes. Researchers often can deduce aspects of the structure of [integral membrane proteins](#) based on the [membrane topology](#) predicted by [hydrophobicity analysis](#). See [protein structure prediction](#).

In the past few years it has become possible for highly accurate physical [molecular models](#) to complement the *in silico* study of biological structures.



especially **proteins** and **nucleic acids**, how they acquire the structures they have, and how alterations in their structures affect their function.

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similarity principle:
geometrically similar molecules are likely to have
similar functions

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Molecule of the Month
HIV Envelope Glycoprotein
 Viruses are faced with a tricky problem: they need to get inside cells, but cells are surrounded by a protective membrane. Enveloped viruses like HIV and influenza, which are themselves surrounded by a similar membrane, solve this problem by fusing with the cell membrane. The envelope glycoprotein (Env) of HIV performs the many complex steps needed for membrane fusion. First, it attaches itself to proteins on the surface of the cell. Then, it acts like a spring-loaded mousetrap and snaps into a new conformation that drags the virus and cell close enough that the membranes fuse. Finally, the HIV genome is released into the cell, where it quickly gets to work building new viruses.

Full Article

Protein Structure Initiative Featured System
Discovering Deaminases
 The function of a protein is implicit in its sequence: if you construct a protein with the proper sequence and provide it an amenable biological environment, it will fold up and start performing its nanoscale task. Many steps of this process, however, hold great mysteries, and predicting this connection between sequence and function is currently a challenge. PSI laboratories in the **Enzyme Function Initiative** have developed an effective pipeline for the prediction of function in bacterial enzymes. An earlier installment of the **PSI Featured System** described one of the early successes: the prediction of function of Tm0936, which turned out to be a deaminase (PDB entry **2plm**). Work has continued on this class of enzymes, and the group recently reported the successful prediction of function in a wide variety of related enzymes.

Full Article | Archive | PSI Structural Biology Knowledgebase

Explore Archive Hide

Organism

Exp. Method

Release Date

Enzyme Classification

Protein Symmetry

Membrane Proteins

Taxonomy

X-ray Resolution

Polymer Type

SCOP Classification

Protein Stoichiometry

Organism

- Homo sapiens (24676)
- Escherichia coli (4815)
- Mus musculus (4214)
- Saccharomyces cerevisiae (2291)
- Bos taurus (2248)
- Rattus norvegicus (2051)
- Escherichia coli K-12 (1841)
- Other (53030)

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Latest release: December 2013

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Winter Newsletter Published

Read about the International Year of Crystallography, data deposition and website statistics for 2013, the 2013 Annual Report, and more.

about 100,000 3D structures of proteins

similarity ppl: also in **chemoinformatics**

Chemical similarity

From Wikipedia, the free encyclopedia

Chemical similarity (or **molecular similarity**) refers to the similarity of [chemical elements](#), [molecules](#) or [chemical compounds](#) with respect to either [structural](#) or functional qualities, i.e. the effect that the chemical compound has on [reaction](#) partners in anorganic or biological settings. Biological effects and thus also similarity of effects are usually quantified using the [biological activity](#) of a compound. In general terms, function can be related to the [chemical activity](#) of compounds (among others).

The notion of *chemical similarity* (or *molecular similarity*) is one of the most important concepts in [chemoinformatics](#).^{[1][2]} It plays an important role in modern approaches to predicting the properties of chemical compounds, designing chemicals with a predefined set of properties and, especially, in conducting drug design studies by screening large databases containing structures of available (or potentially available) chemicals. These studies are based on the similar property principle of Johnson and Maggiora, which states: *similar compounds have similar properties*.^[1]

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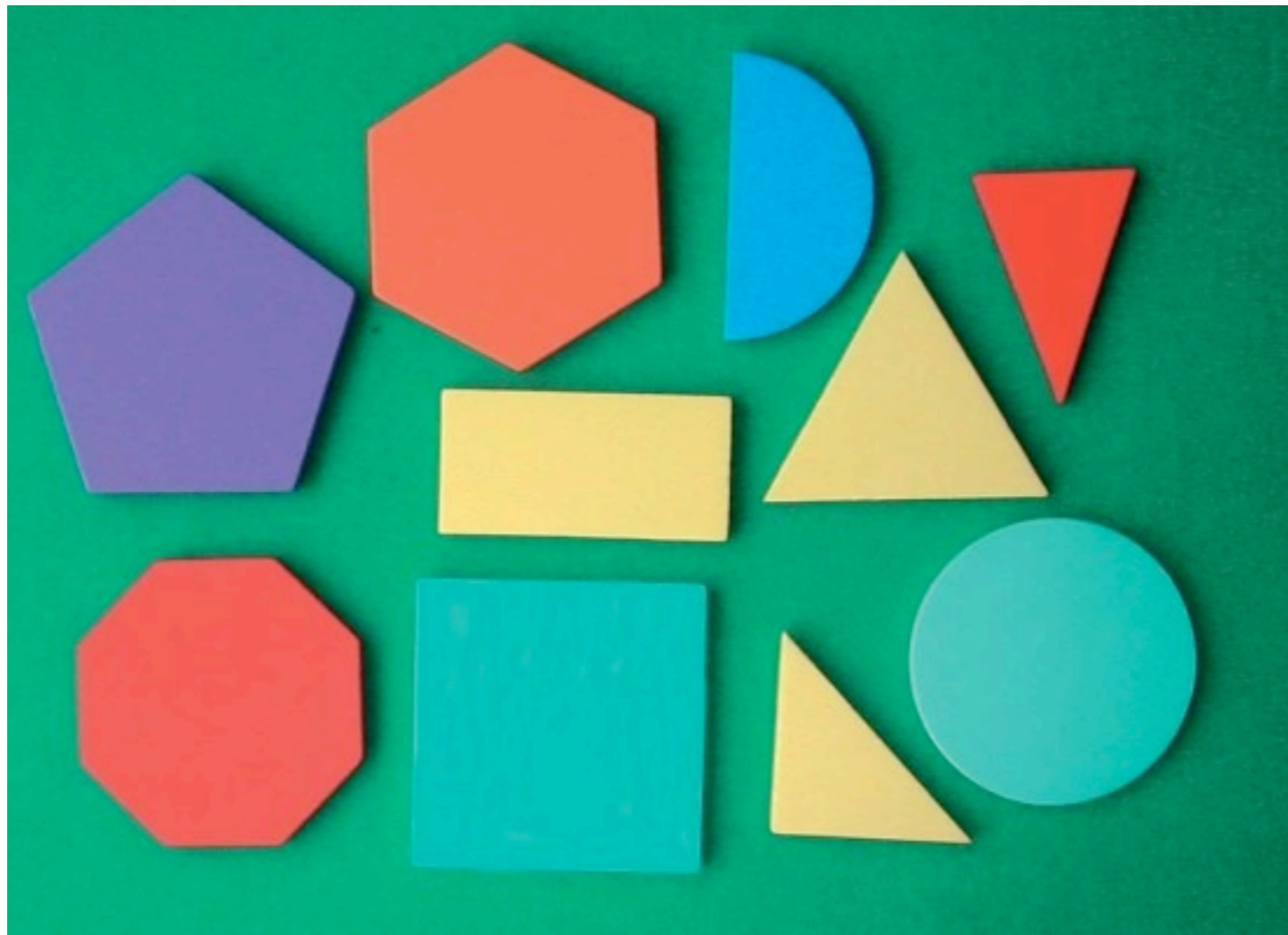
Cheminformatics

From Wikipedia, the free encyclopedia

(Redirected from [Chemoinformatics](#))

Cheminformatics (also known as **chemoinformatics**, **chemioinformatics** and **chemical informatics**) is the use of computer and [informational](#) techniques applied to a range of problems in the field of [chemistry](#). These *in silico* techniques are used in, for example, [pharmaceutical](#) companies in the process of [drug discovery](#). These methods can also be used in chemical and allied industries in various other forms.

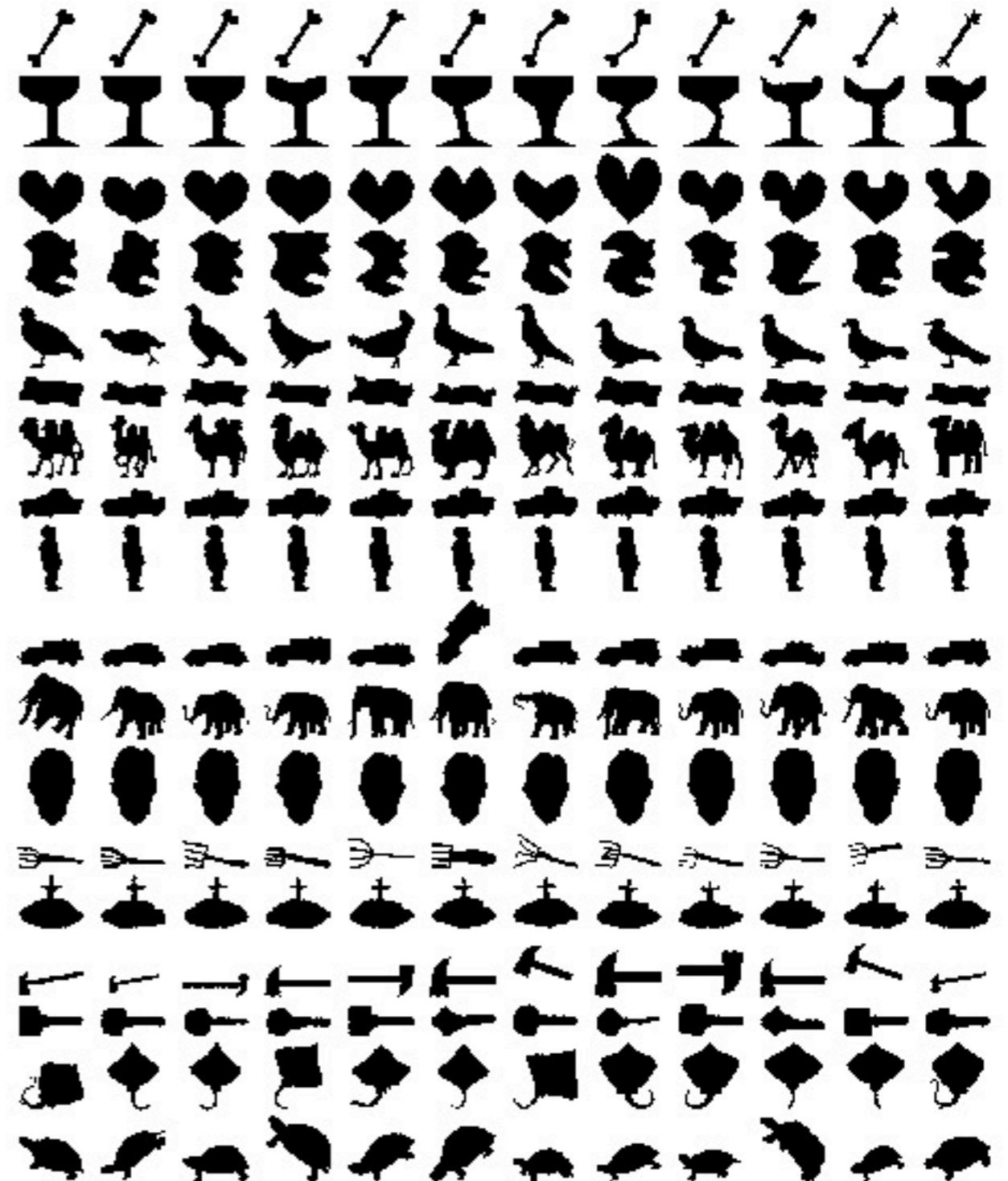
2d shapes...



2d shapes...



MNIST db: handwritten text recognition -- think USPS



segmented real objects -- MPEG 7 db



MNIST database

From Wikipedia, the free encyclopedia

The **MNIST database** (Mixed [National Institute of Standards and Technology](#) database) is a large [database](#) of handwritten digits that is commonly used for training various [image processing](#) systems.^{[1][2]} The database is also widely used for training and testing in the field of [machine learning](#).^{[3][4]} It was created by "re-mixing" the samples from NIST's original datasets. The creators felt that since NIST's training dataset was taken from [American Census Bureau](#) employees, while the testing dataset was taken from [American high school](#) students, NIST's complete dataset was too hard.^[5] Furthermore, the black and white images from NIST were [normalized](#) to fit into a 20x20 pixel bounding box and [anti-aliased](#), which introduced grayscale levels.^[5]

The database contains 60,000 training images and 10,000 testing images.^[6] Half of the training set and half of the test set were taken from NIST's training dataset, while the other half of the training set and the other half of the test set were taken from NIST's testing dataset.^[7] There have been a number of [scientific papers](#) on attempts to achieve the lowest error rate; one paper, using a hierarchical system of [convolutional neural networks](#), manages to get an [error rate](#) on the MNIST database of 0.23 percent.^[8] The original creators of the database keep a list of some of the methods tested on it.^[5] In their original paper, they use a [support vector machine](#) to get an error rate of 0.8 percent.^[9] Recently, an error rate of 0.27% was reported by researchers using a similar system of neural networks.^[10]

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The **MNIST database** (Mixed **N**ational **I**nstitute of **S**tandards and **T**echnology database) is a large **database** of handwritten digits that is commonly used for training various **image processing** systems.^{[1][2]} The database is also widely used for training and testing in the field of **machine learning**.^{[3][4]} It was created by "re-mixing" the samples from NIST's original datasets. The creators felt that since NIST's training dataset was taken from American **Census Bureau** employees, while the testing dataset was taken from **American high school** students, NIST's complete dataset was too hard.^[5] Furthermore, the black and white images from NIST were **normalized** to fit into a 20x20 pixel bounding box and **anti-aliased**, which introduced grayscale levels.^[5]

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Data for MATLAB hackers

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Handwritten Digits

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- USPS Handwritten Digits [[data/usps_all.mat](#)]
 - [pictures: 0 1 2 3 4 5 6 7 8 9]
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- Binary Alphanumerics [[data/binaryalphadigs.mat](#)] [[picture](#)]
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 - From Simon Lucas' (smi@essex.ac.uk), [Algoval](#) system.

Faces

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- Olivetti Faces [[data/olivetti/aces.mat](#)] [[picture](#)]

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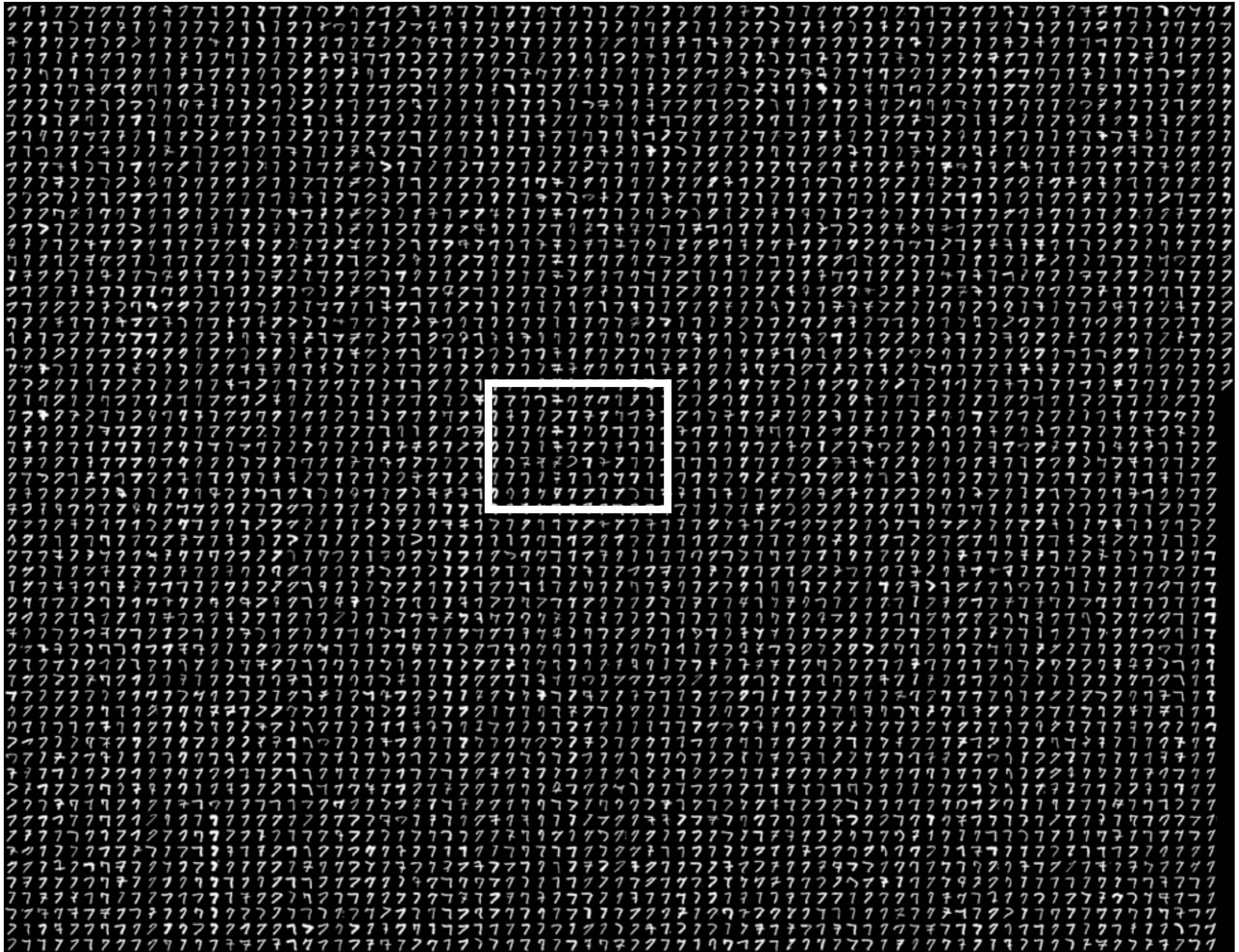
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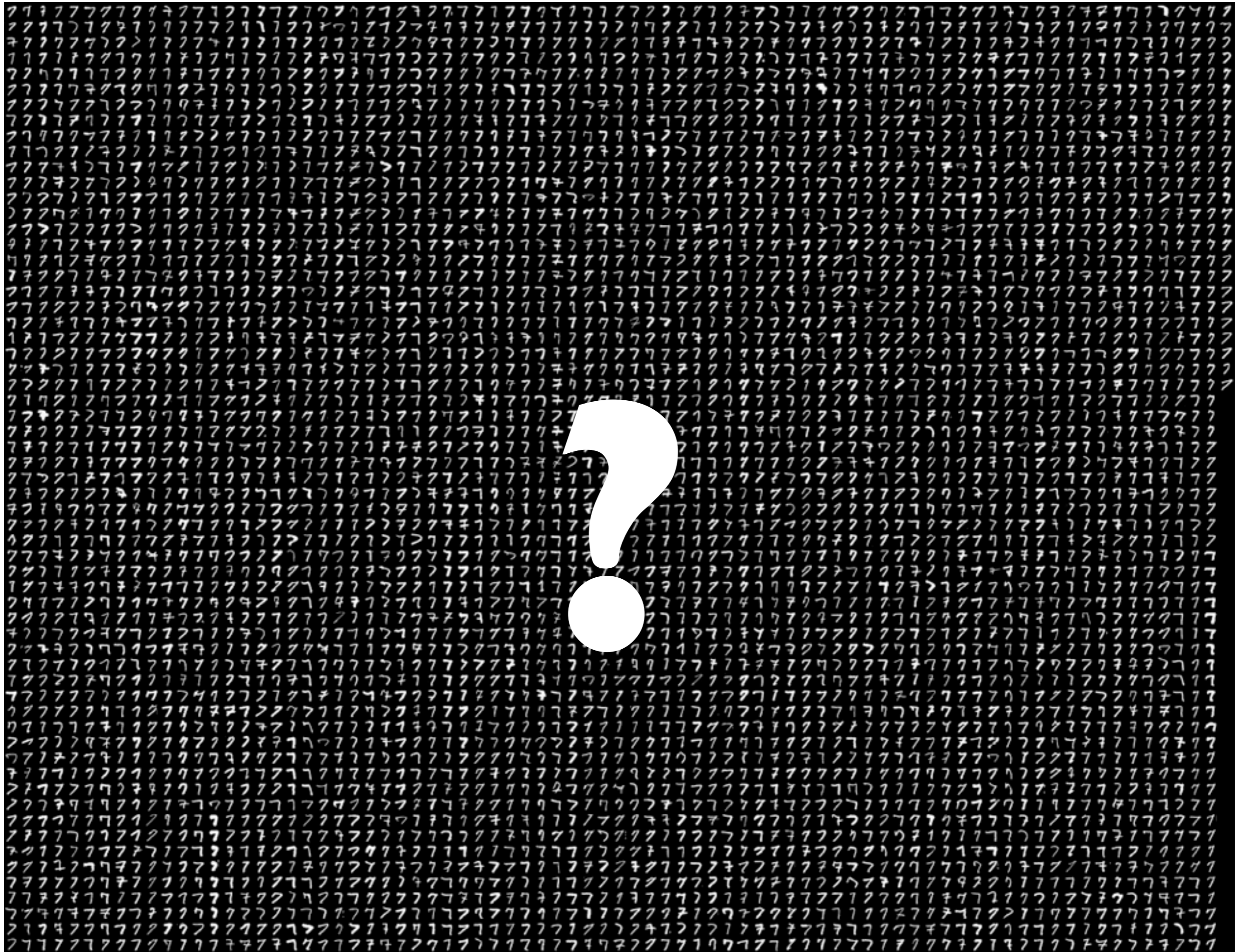
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Monday, January 13, 2014





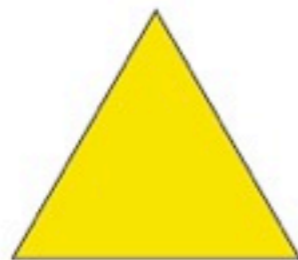
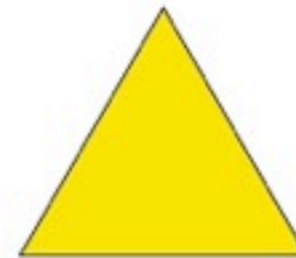




Name _____

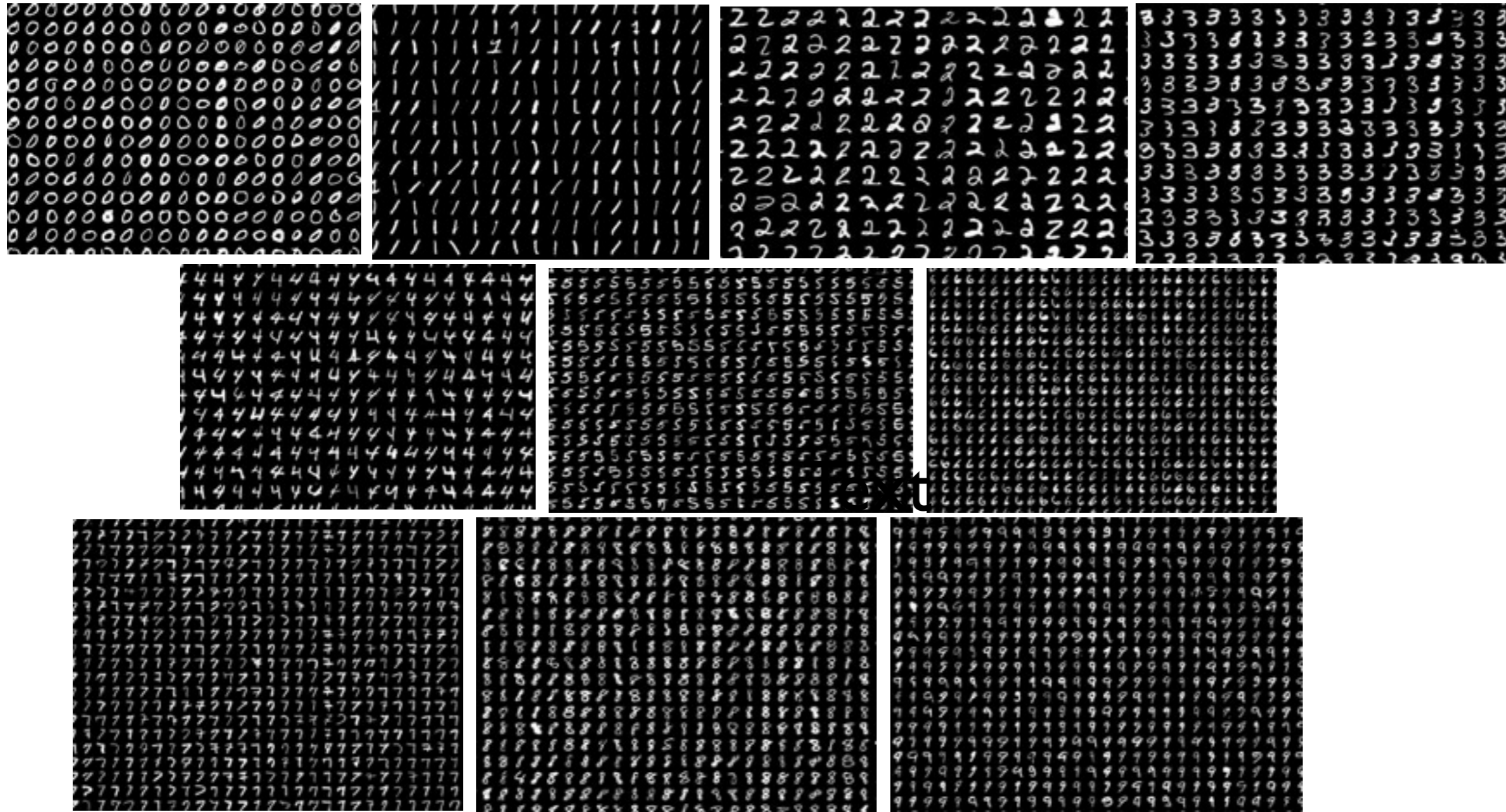
Shape Matching Worksheet

Draw a line from each shape on the left to the matching shape on the right side of the page.

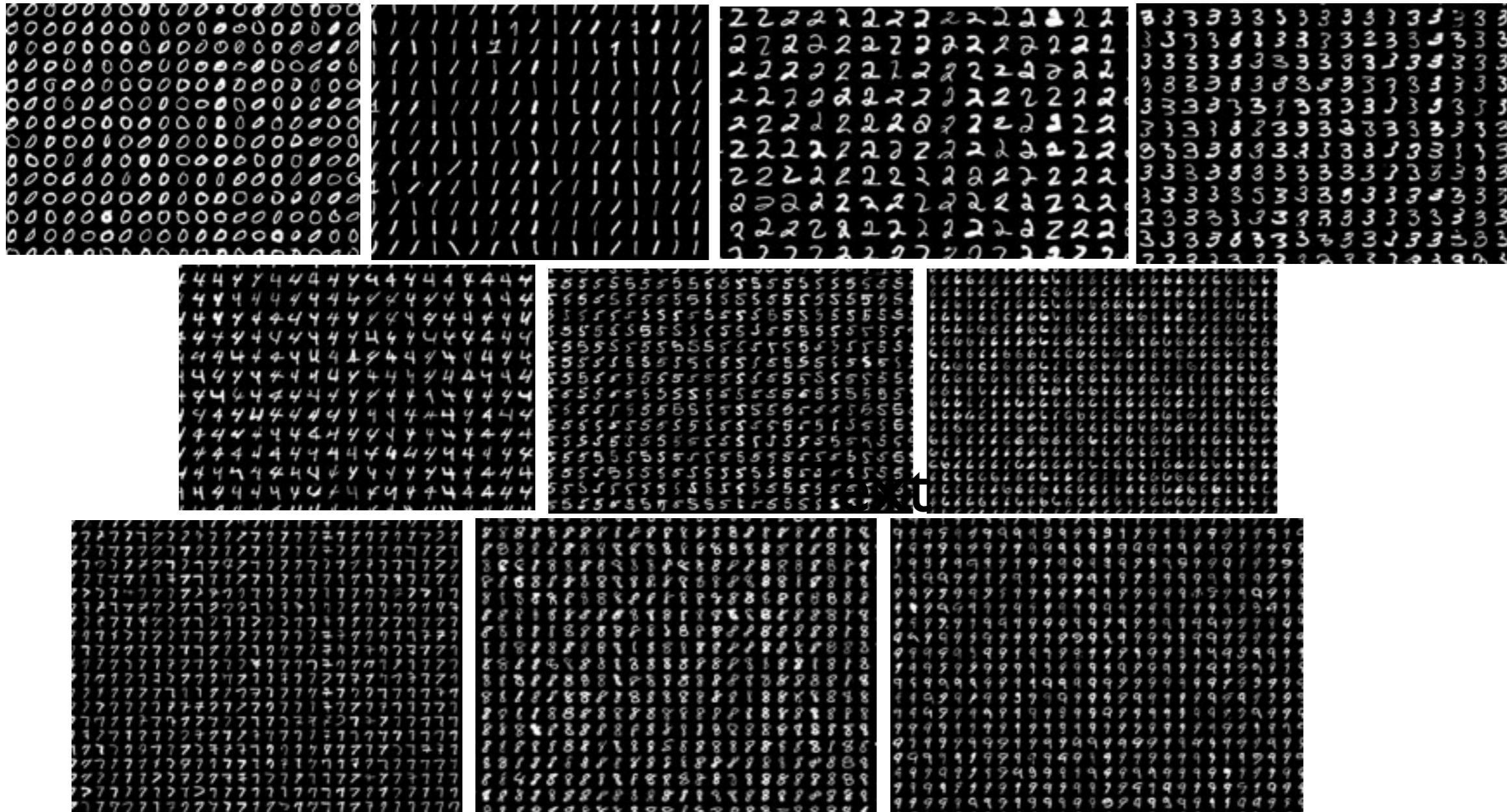


- We intuitively know when two shapes are similar, and how similar they are...
- This intrinsic understanding permits *grouping/classifying* shapes..
- if confronted with zillions of shapes: how do we do that? need a computer...
- How can we extract/define a notion of similarity between shapes that can be used by a computer?

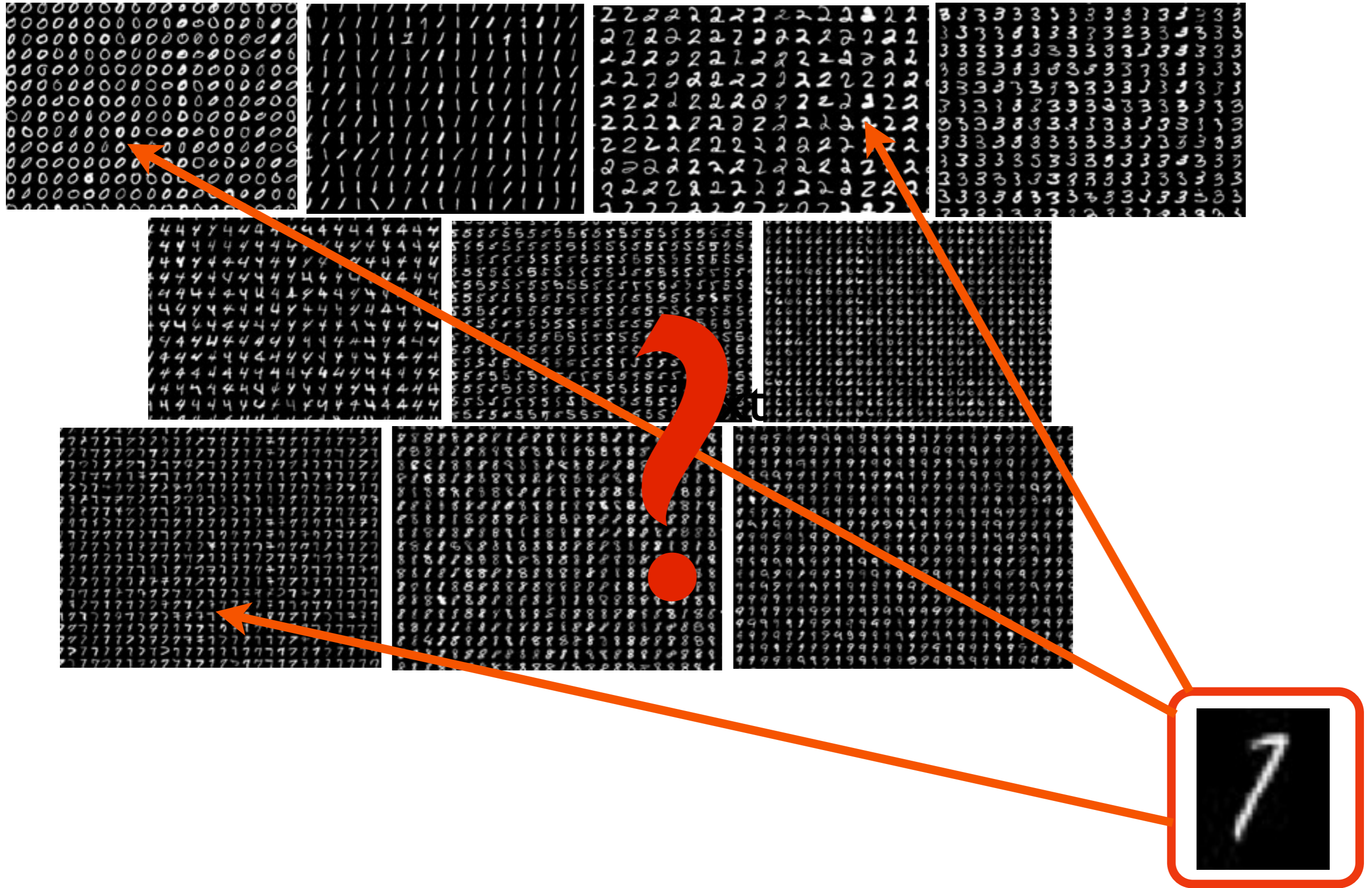
typical scenario



typical scenario



typical scenario



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, \dots, 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} :

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

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

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

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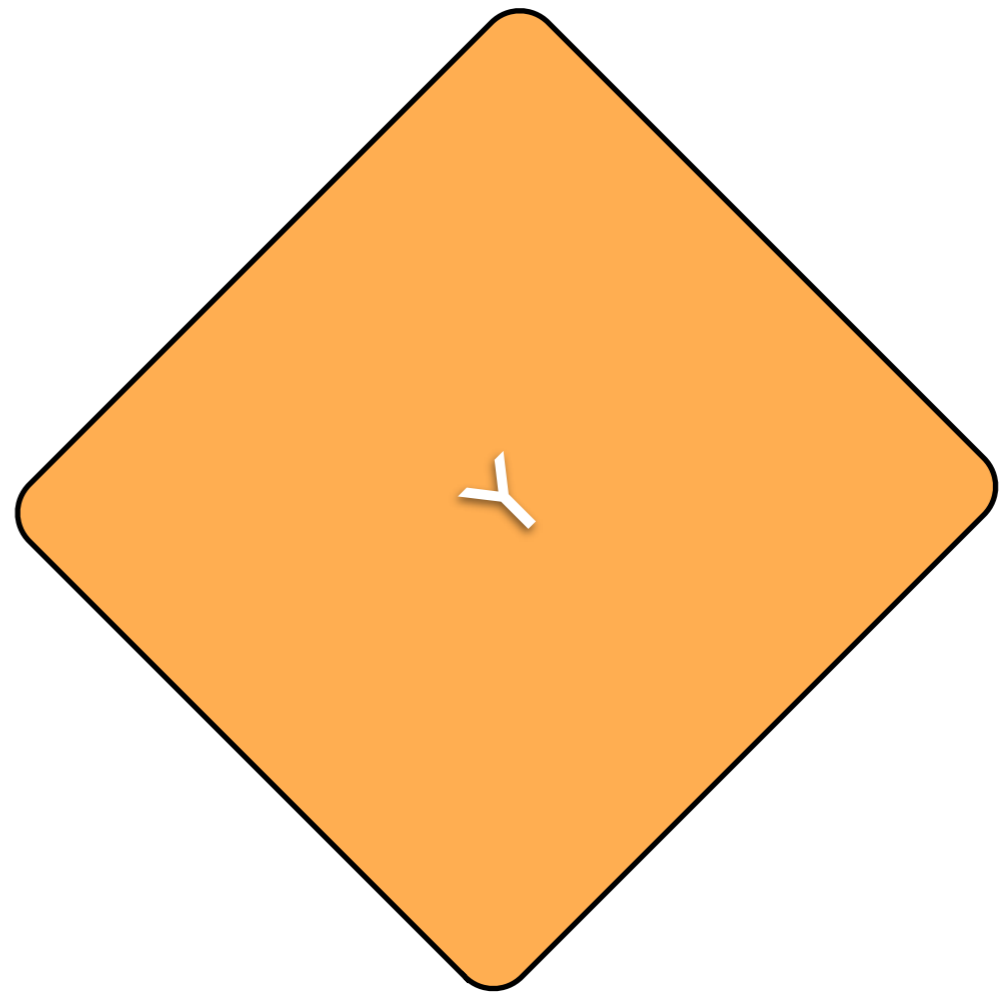
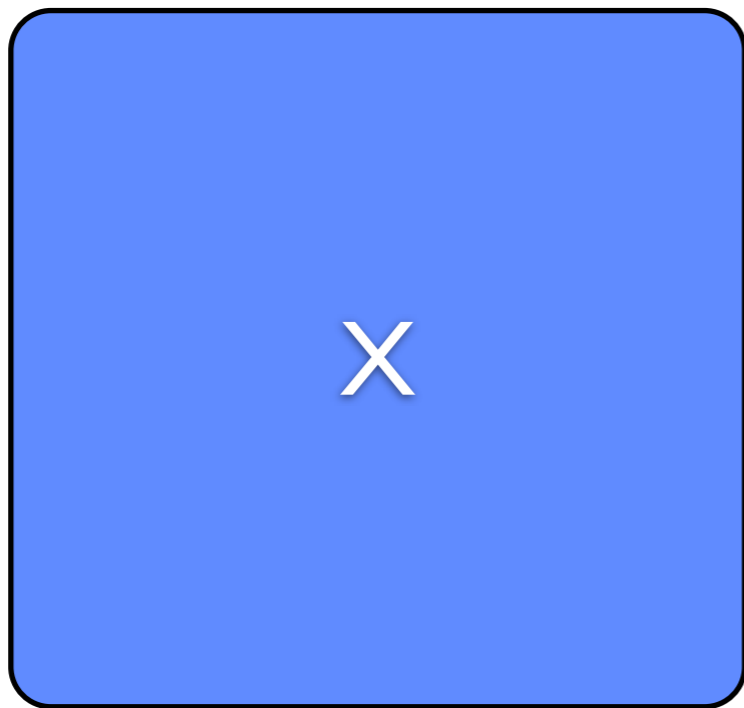
- in order to do this, one first needs to define a notion **dist** of *distance* or *dis-similarity* between objects.

So.. first thing we need: a distance between shapes!

- what is, mathematically, a suitable distance between shapes?
- what properties are important?
- we probably want to be able to compute this distance easily .. computational cost..

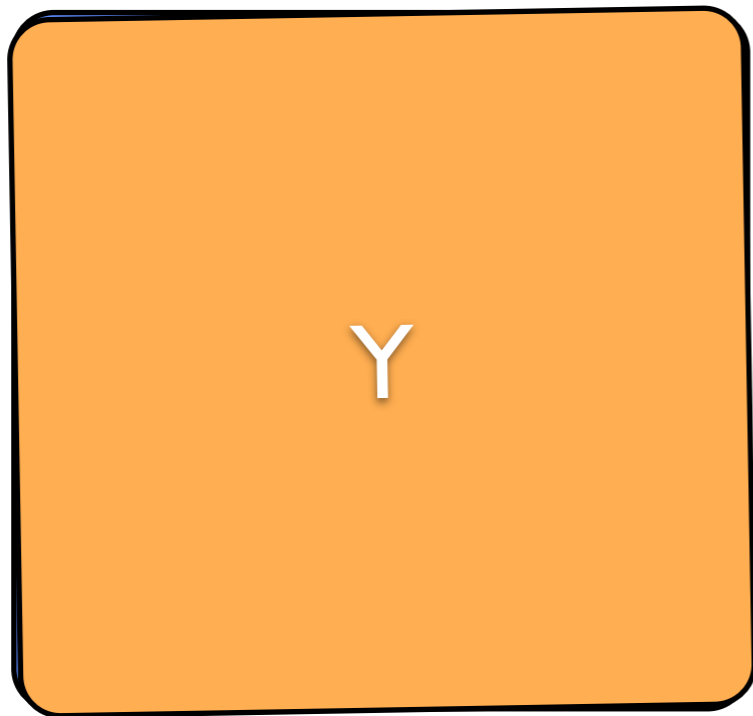
Another important point: invariances

Are these two objects the same?



Another important point: invariances

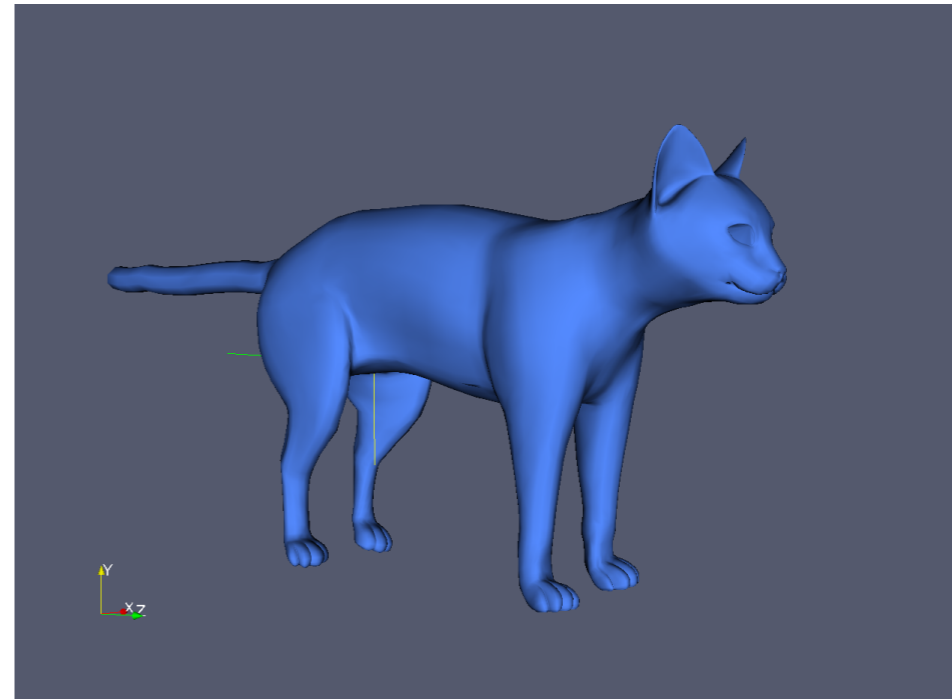
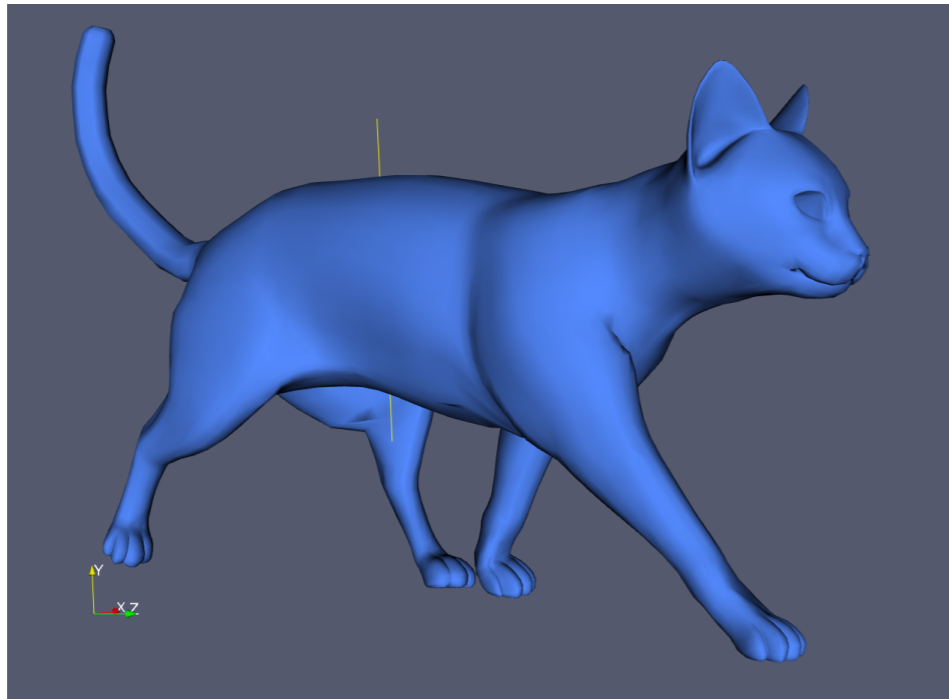
Are these two objects the same?



this is called invariance to *rigid transformations*

Another important points: invariances

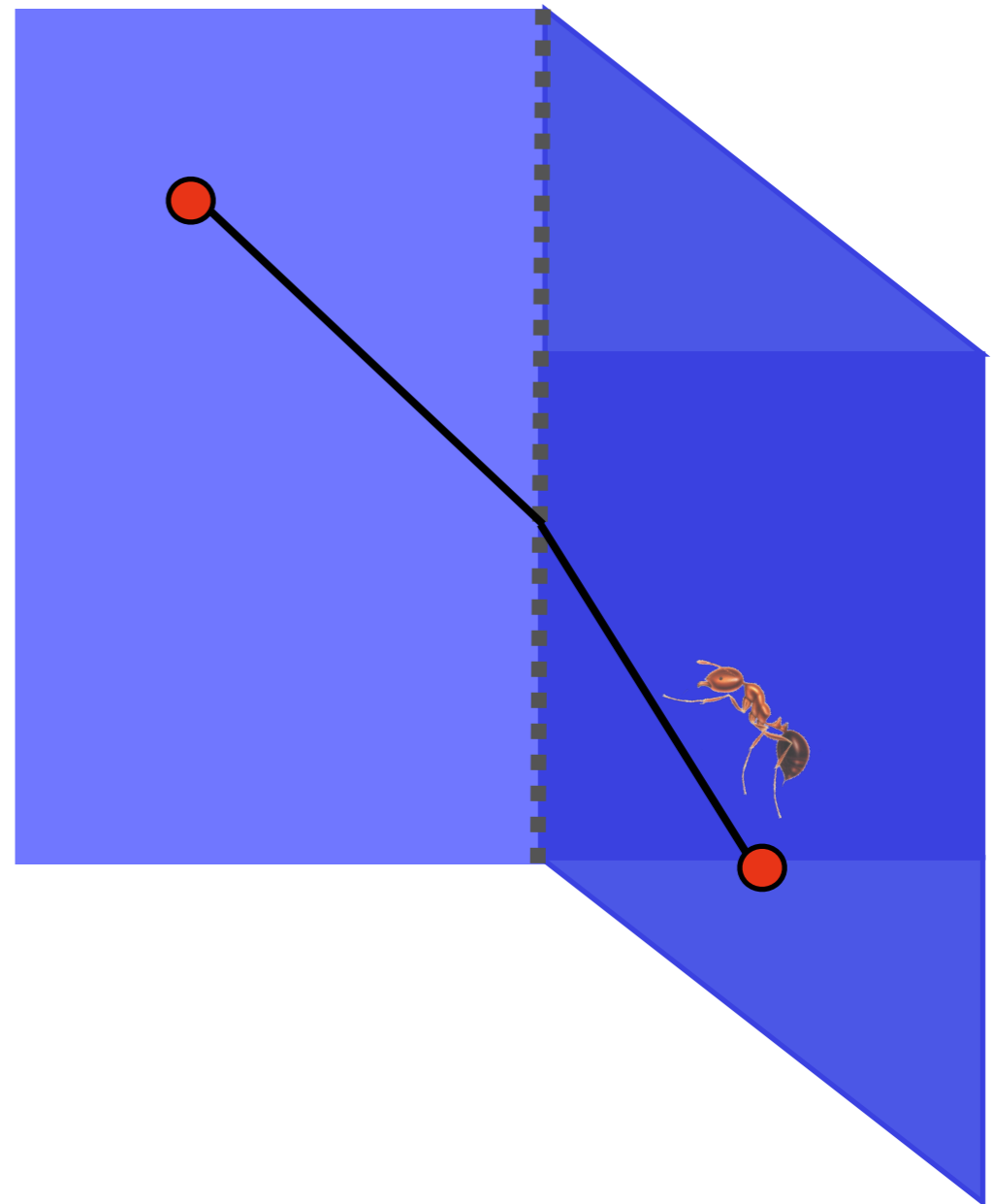
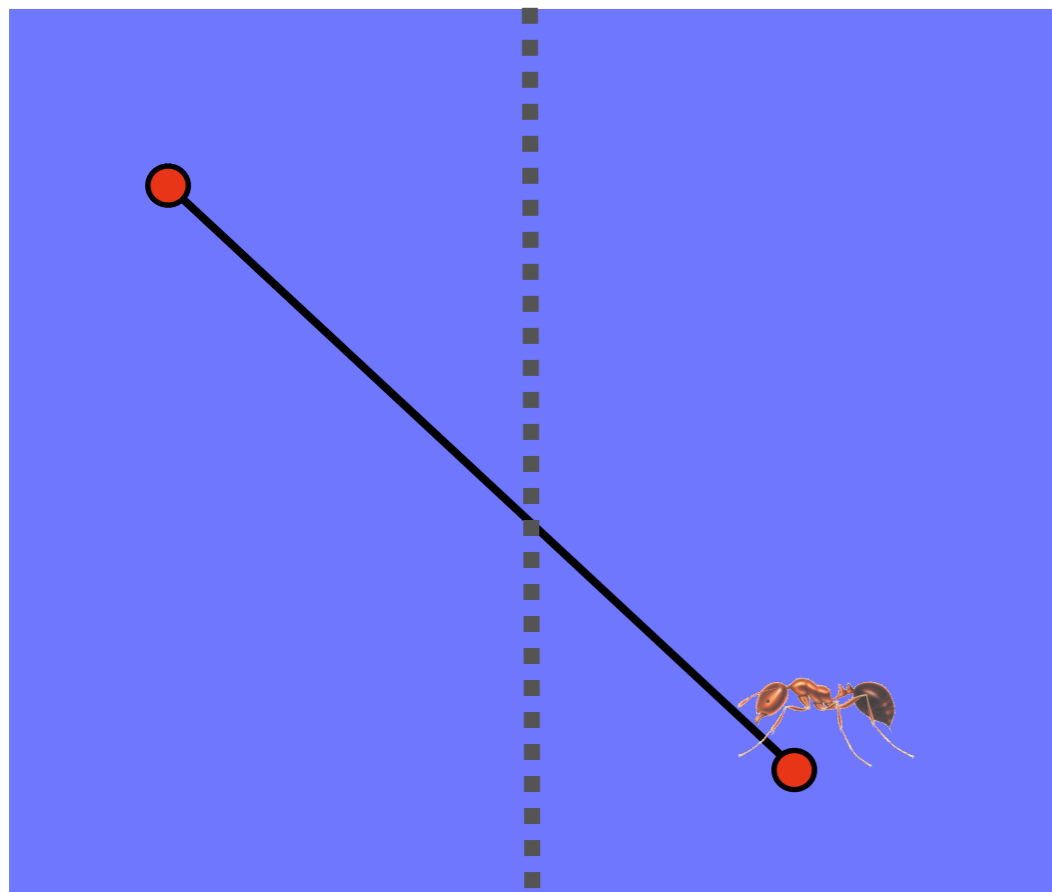
what about these two?



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

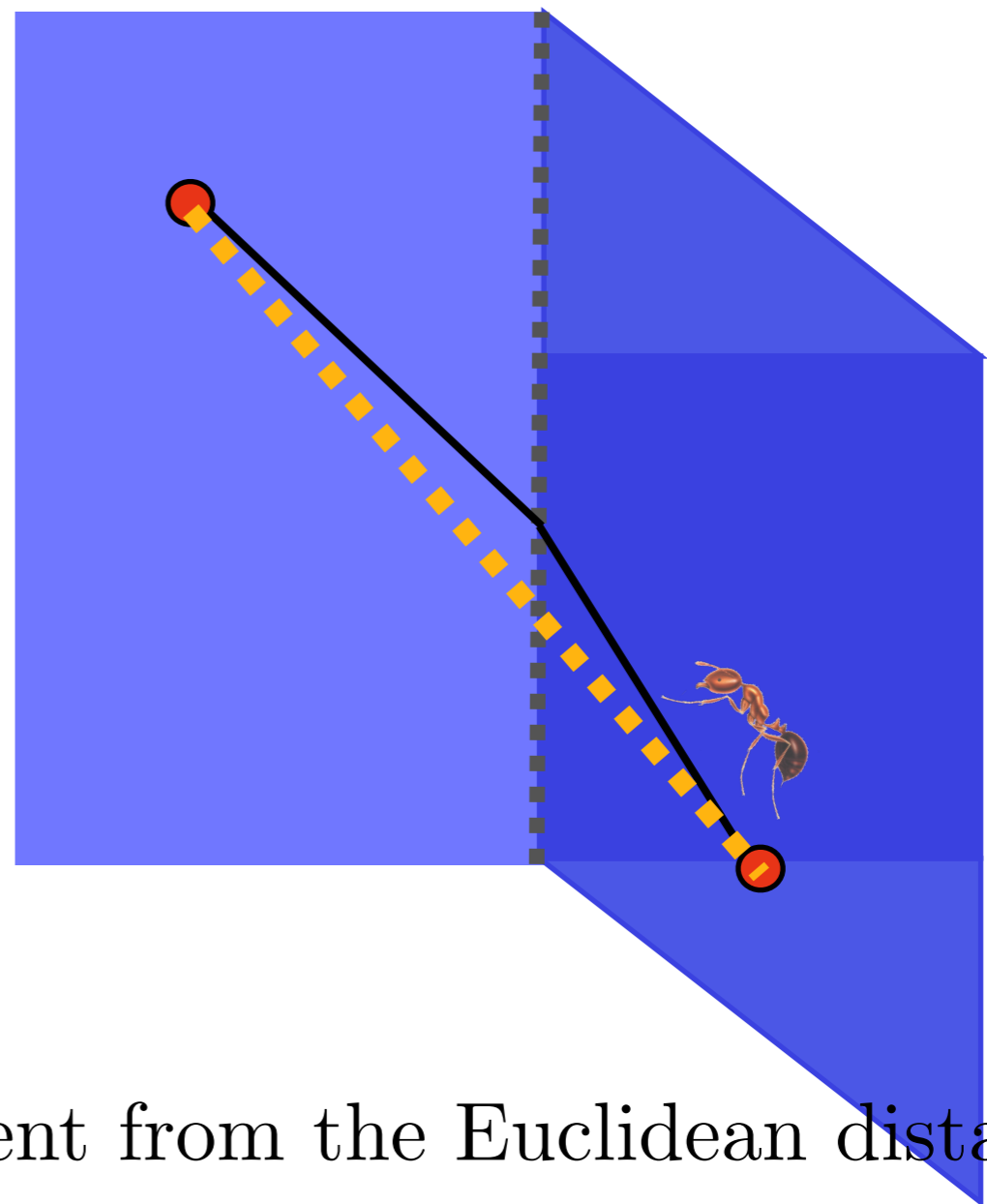
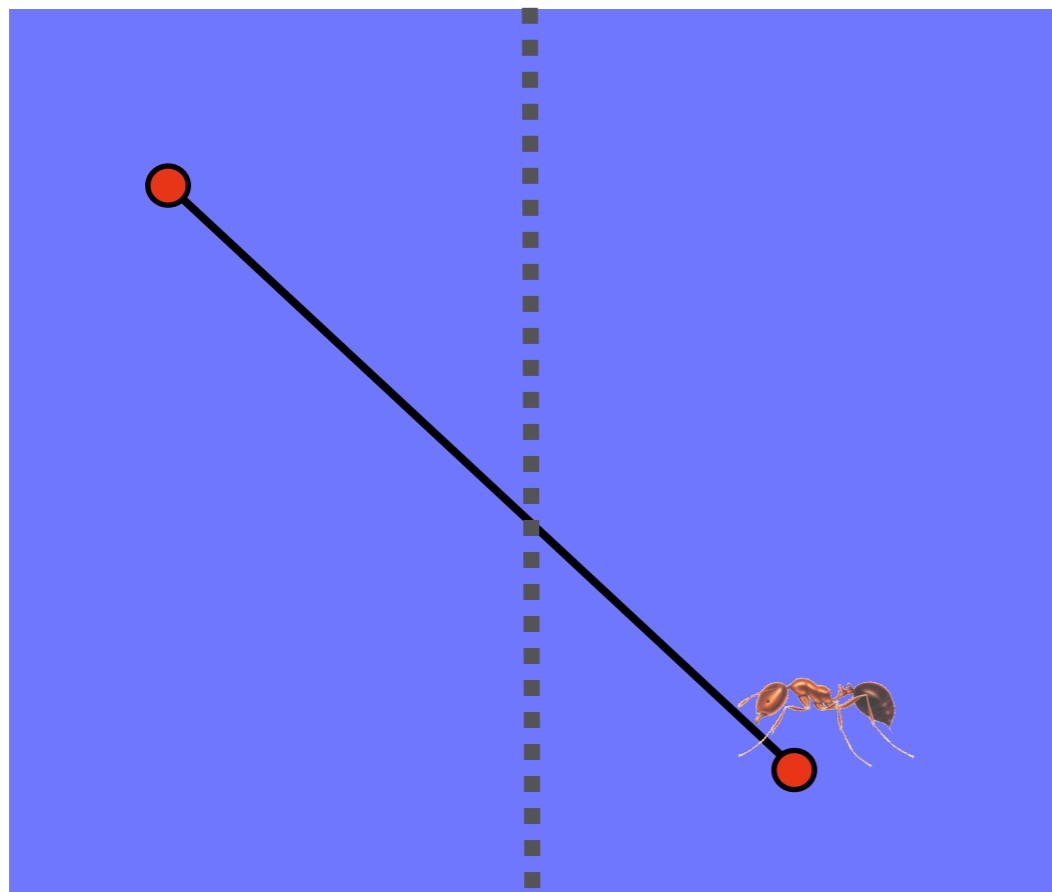
Bending transformations

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

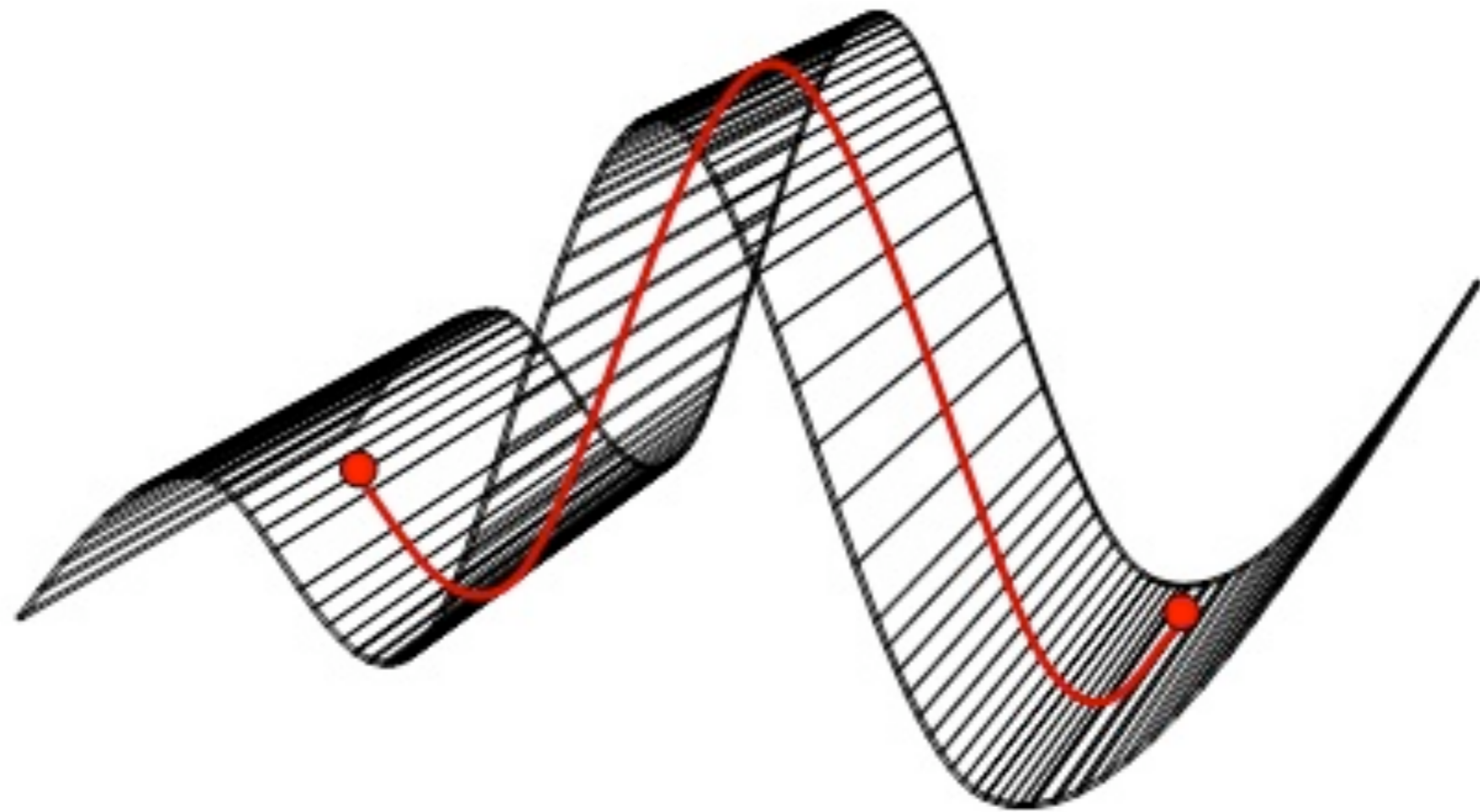


Bending transformations

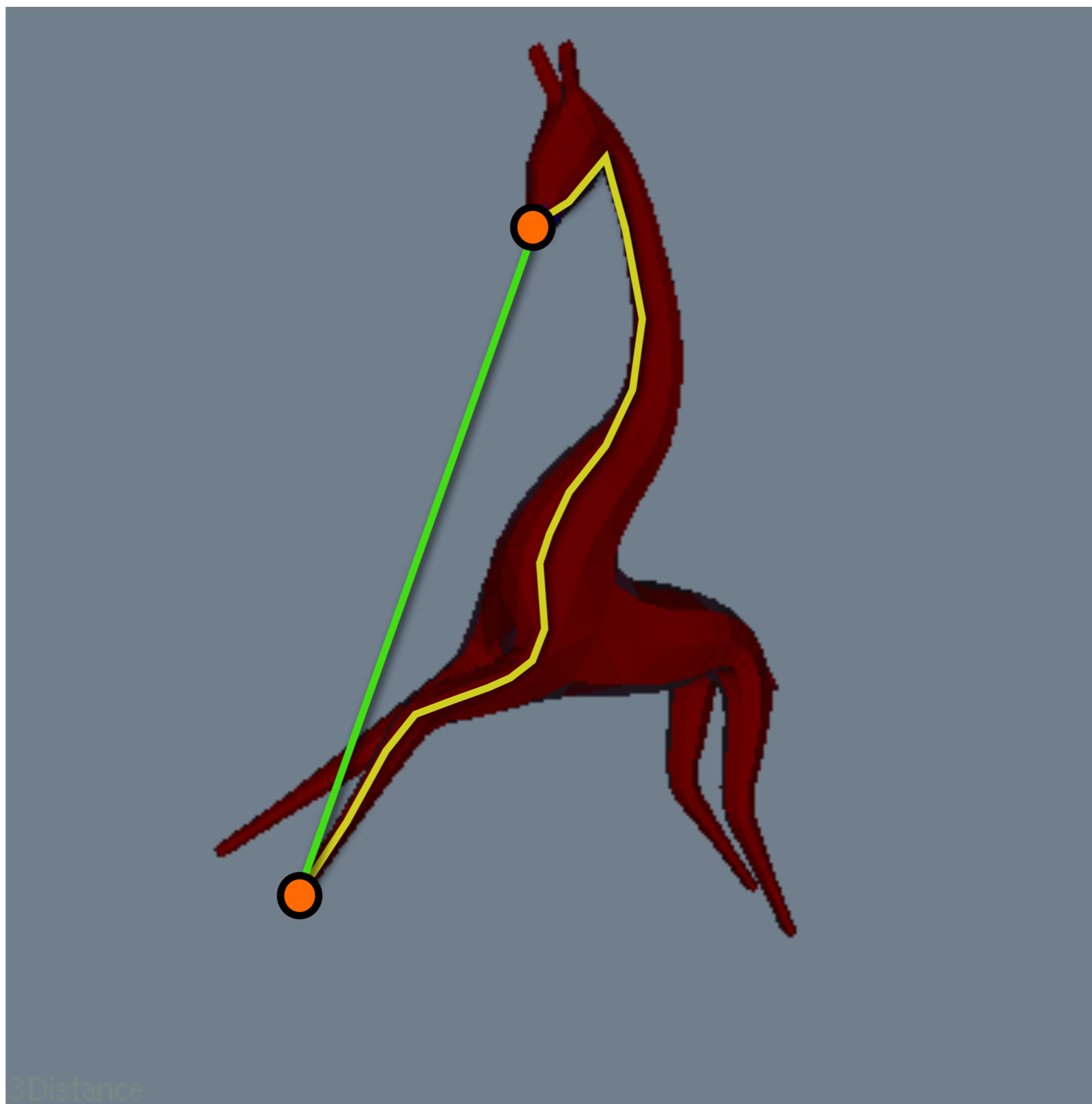
the distance, as measured by an ant, does not change



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



Geodesic distance vs Euclidean distance

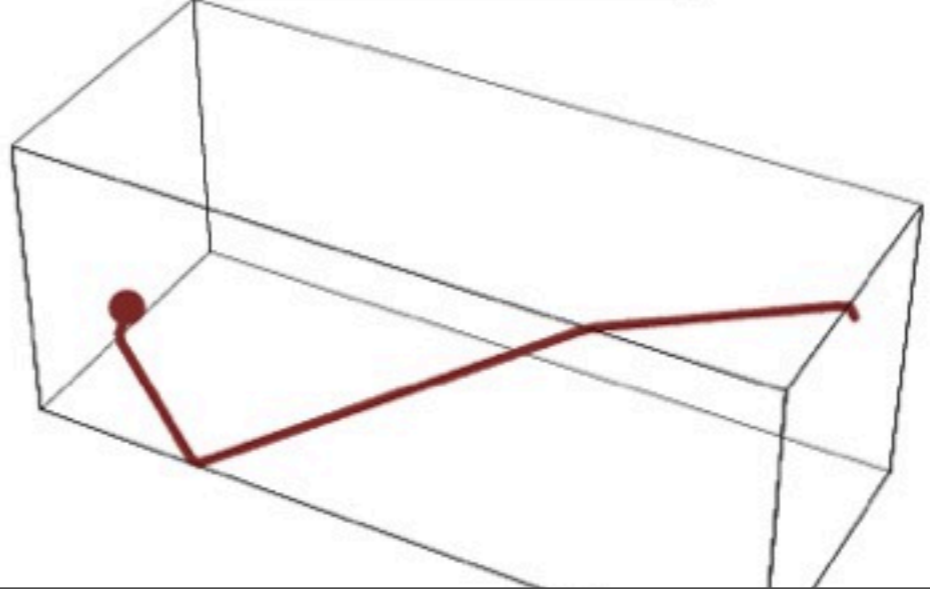
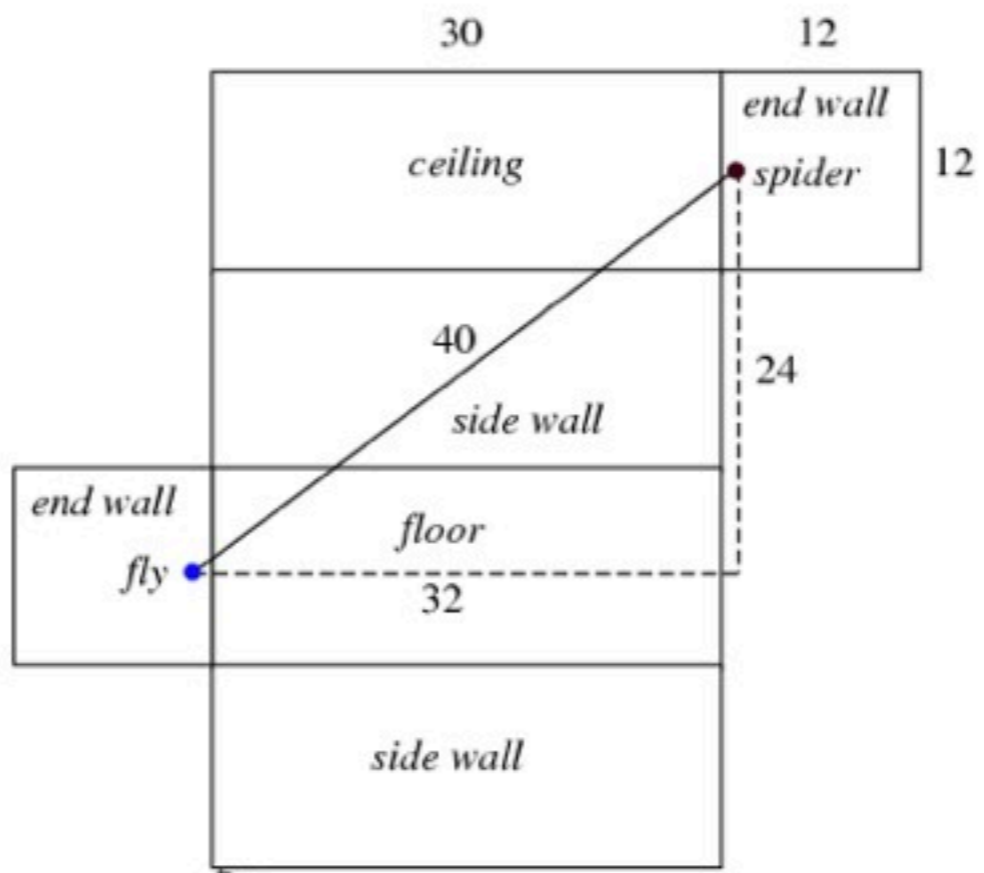


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Spider and Fly Problem

 [DOWNLOAD Mathematica Notebook](#)



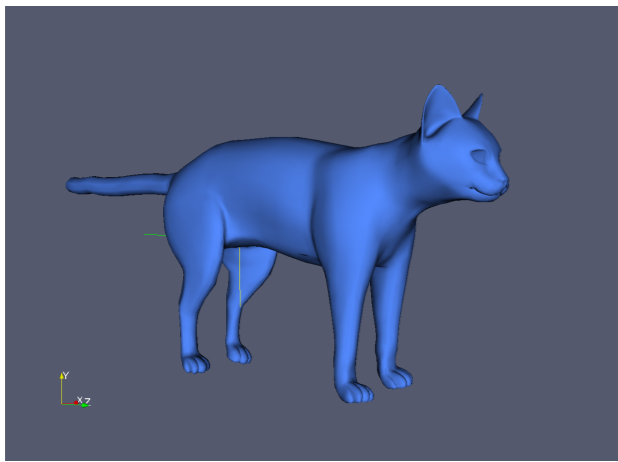
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13,194 entries
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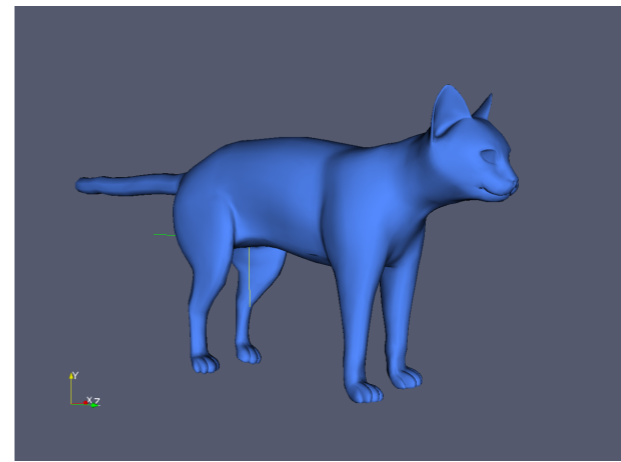
Created, developed, and nurtured by Eric Weisstein at Wolfram Research

invariances...

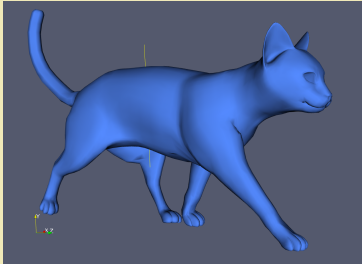
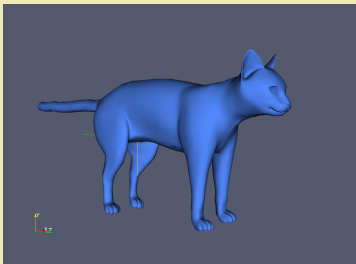
The measure of dis-similarity **dist** must capture the type of invariance you want to encode in your classification system.



=



?

dist ( , ) = 0 ?

A **Metric Space** is a pair (X, d) where X is a set and $d : X \times X \rightarrow \mathbb{R}^+$, 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.*



Metric Geometry in Shape Matching..

What is Metric Geometry?

What is Metric Geometry?

MG is the world of metric spaces..

What is Metric Geometry?

MG is the world of metric spaces..

what can I say about the geometry of a shape/space using only measurements of distance?

Example/Exercise



You land in a new planet (perfect sphere). You find no-one around.. how do you estimate the (size) radius of the planet?

Say you only have a (short) measuring tape..



Summary

- Shapes are being produced at a fast pace. We need methods for organizing collection of shapes.
- 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).
- We will model this dis-similarity as a metric or distance between objects – metric space structure!