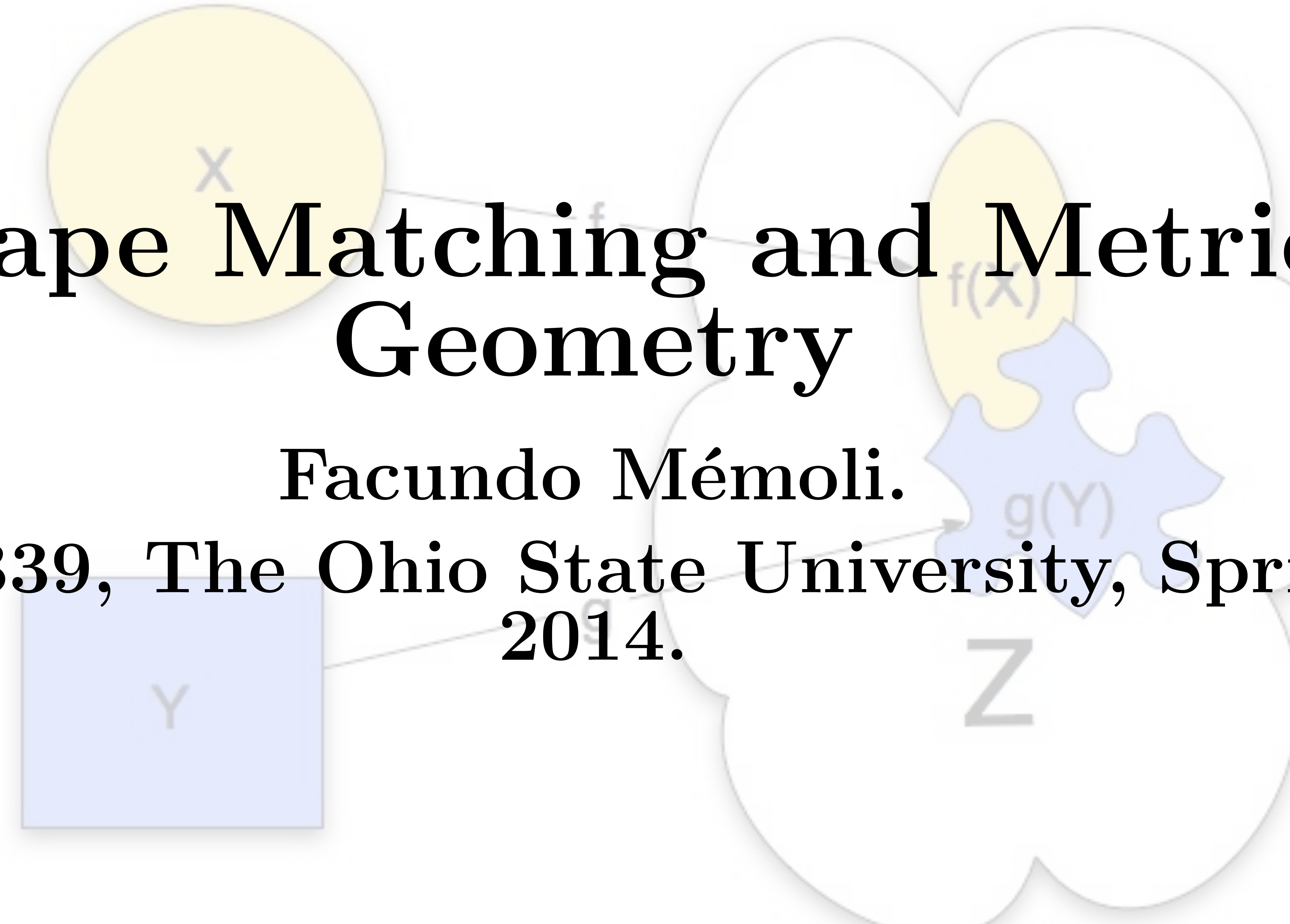
Shape Matching and Metric Geometry

Facundo Mémoli.

CS 5339, The Ohio State University, Spring 2014.



https://people.math.osu.edu/memoli.2/courses/cse-topics-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

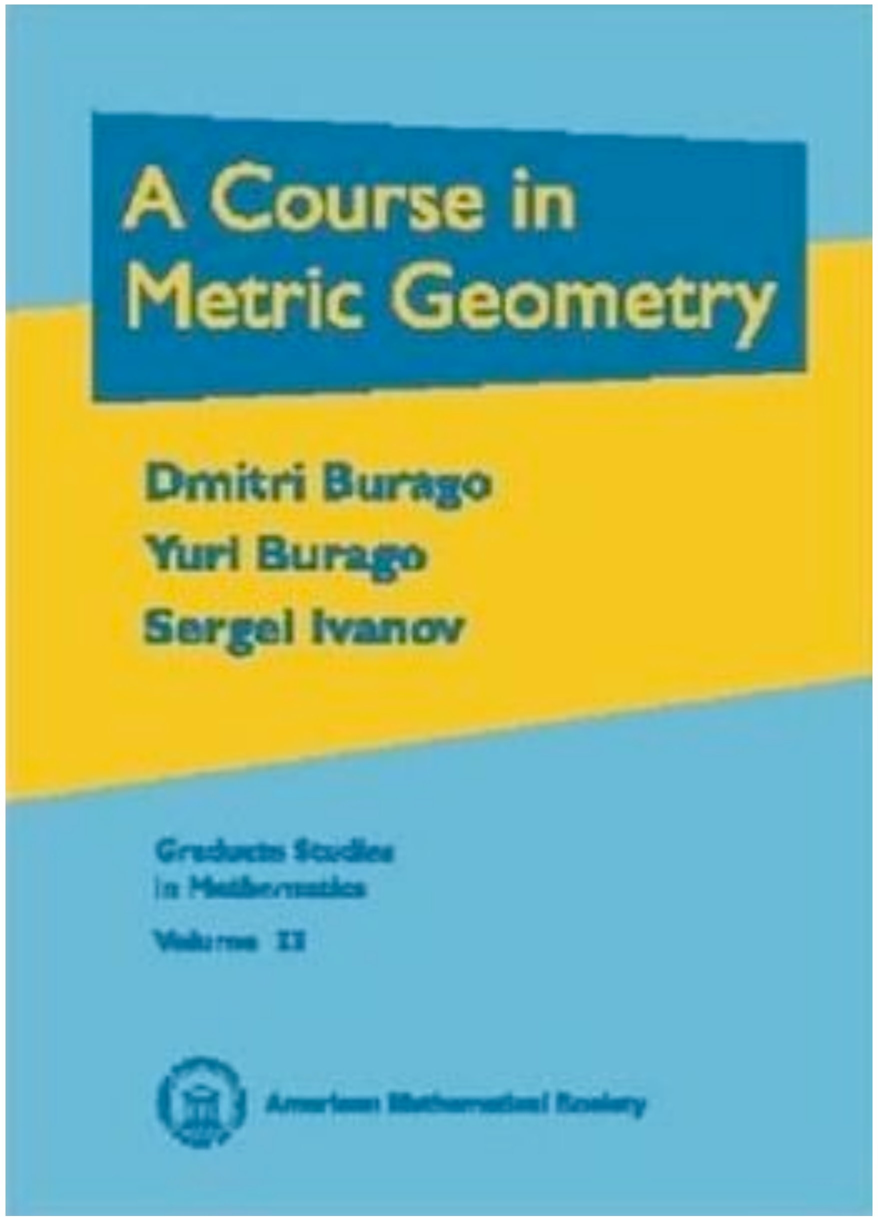
The grade will be based on three components. Everyone will be involved in (1) presenting paper(s) and in (2) a final project. The project will be based on reading a number of papers and then presenting them in class and writing up a report. Topics and emphasis will depend on the interest of each student. 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.

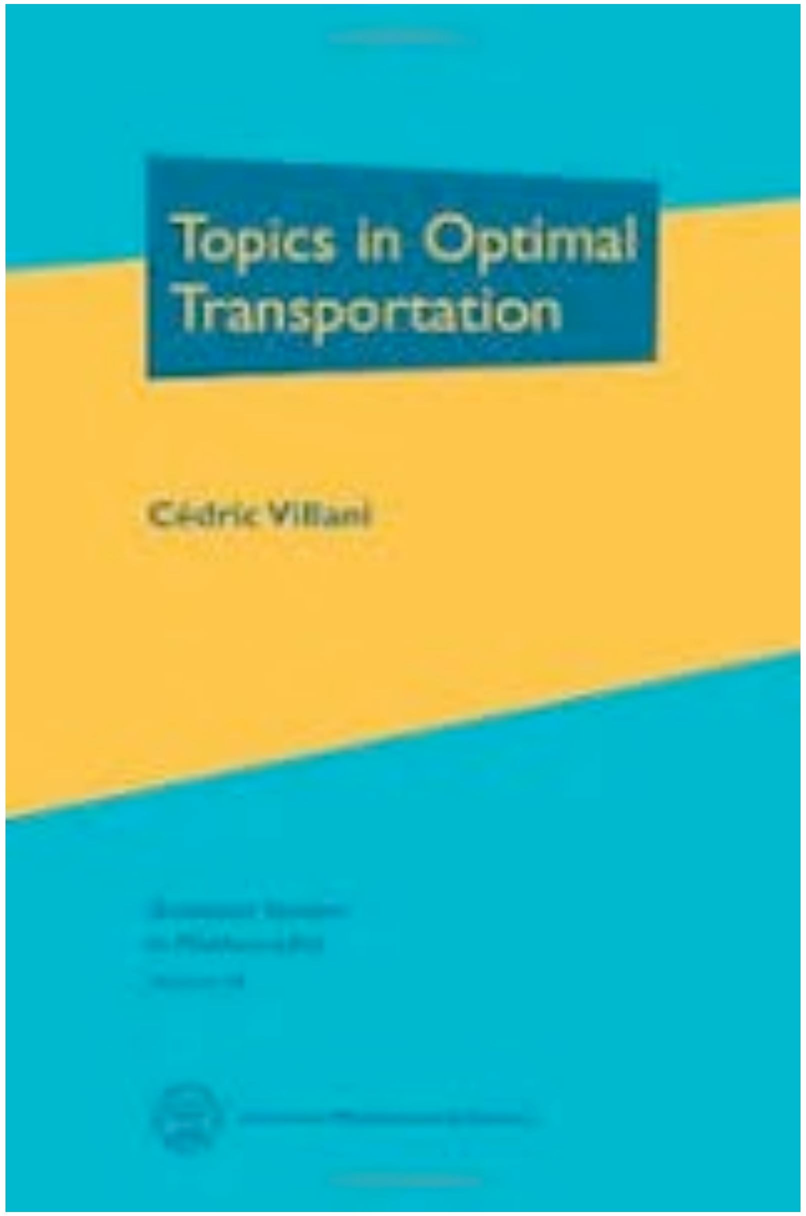
office hours etc

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

a couple of reference books:



[BBI]



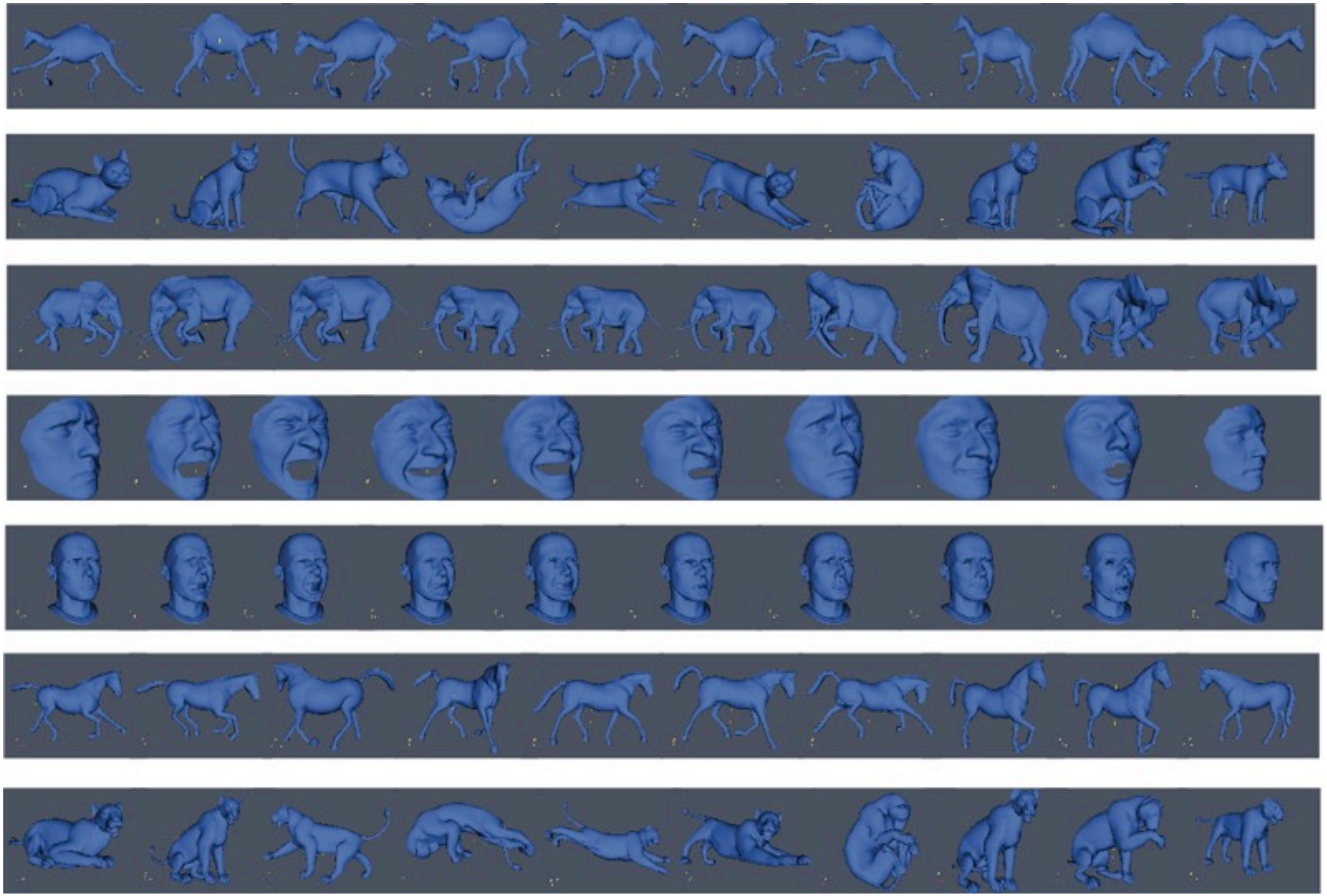
[Villani]

Note: these are **not** textbooks

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

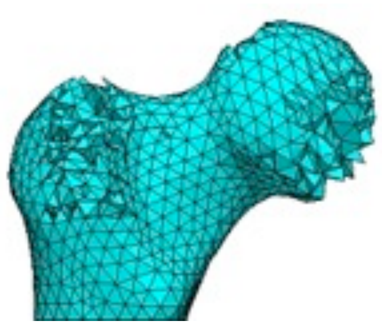
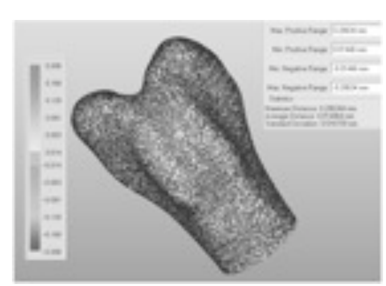
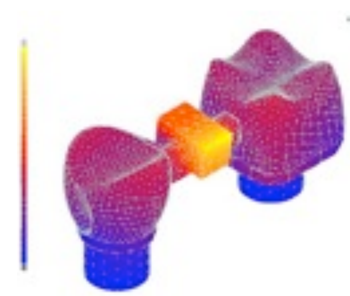
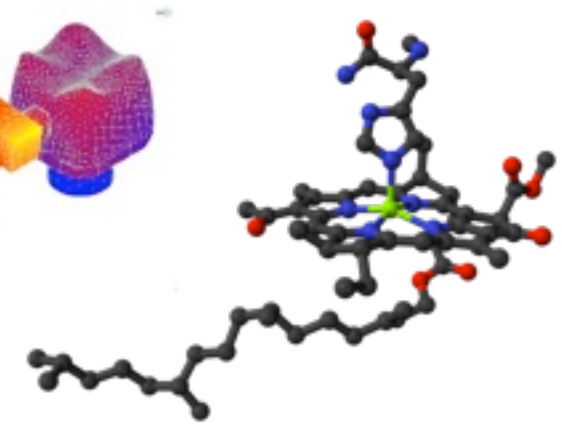
The Problem of Shape/Object Matching

- 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 protheses
  - text documents
  - more complicated structures present in datasets (things you can't visualize)



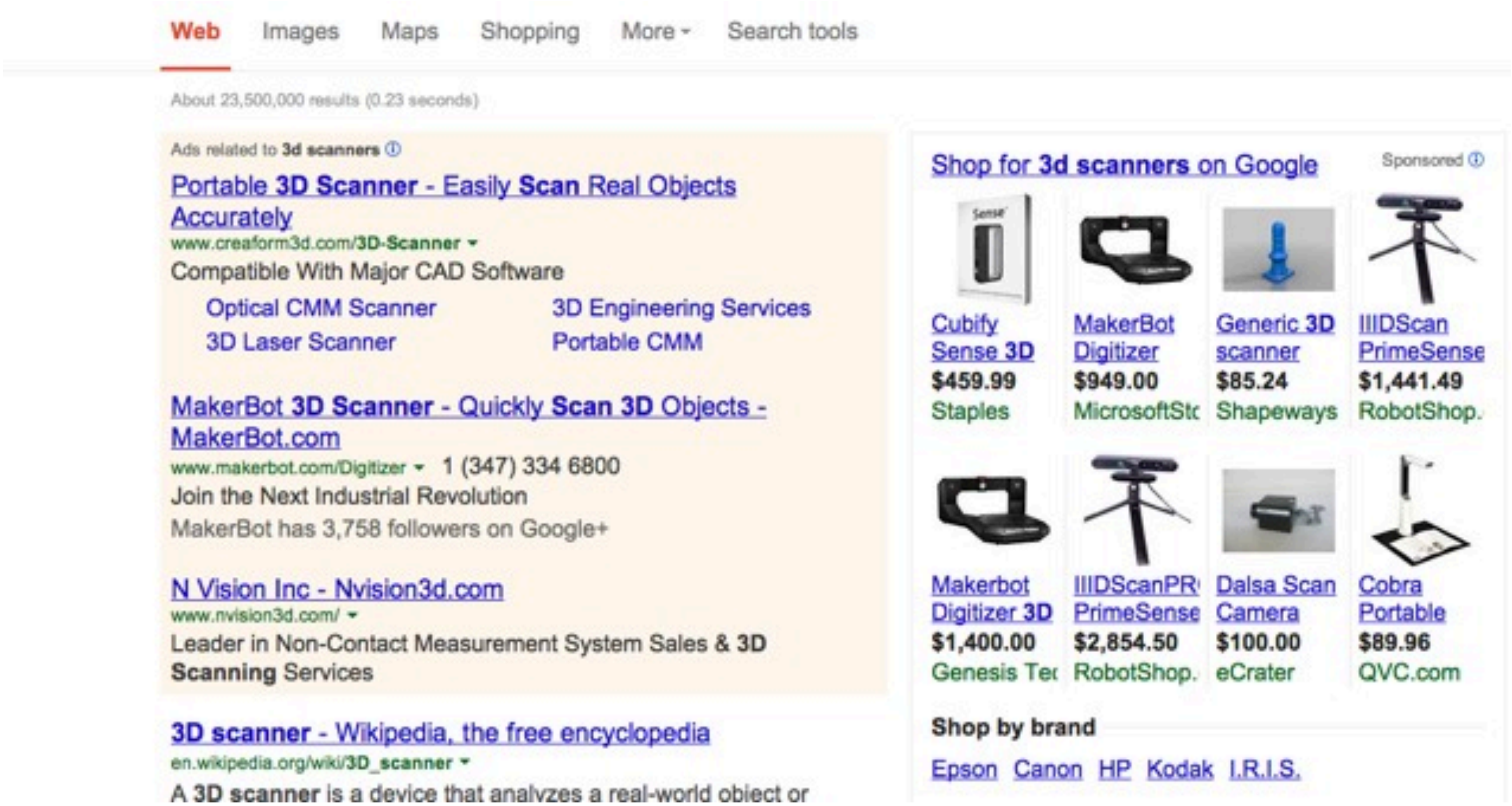
3D objects: examples

- 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`

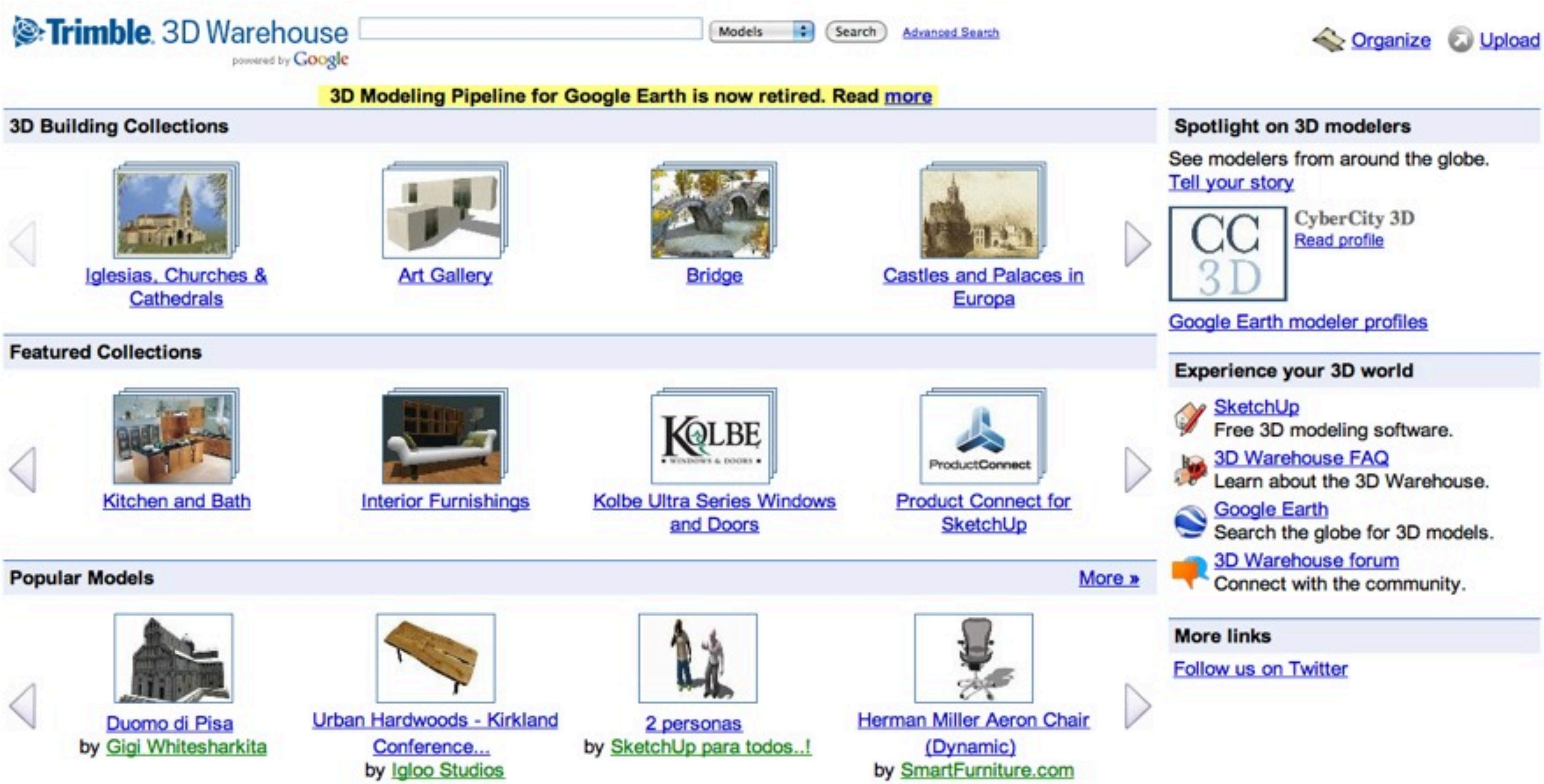







- 3D scanners are becoming increasingly cheaper.
- consequence: lots of 3D data are being generated and stored.
- 3D printing!

- How do we organize those datasets?



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



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

https://graphics.stanford.edu/projects/mich/

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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The first deadline for submissions is December 31!
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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."

The *CyArk* logo.

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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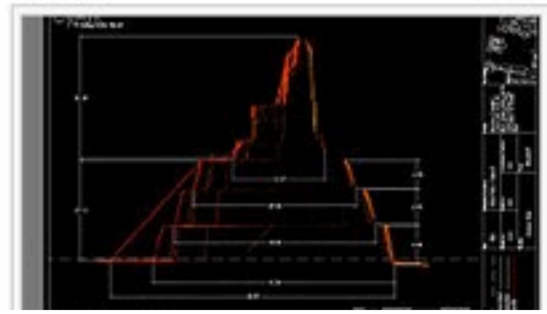
History [edit]



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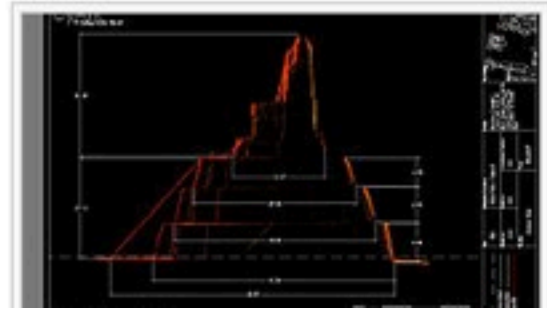

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Ben Kacyra: Ancient wonders captured in 3D

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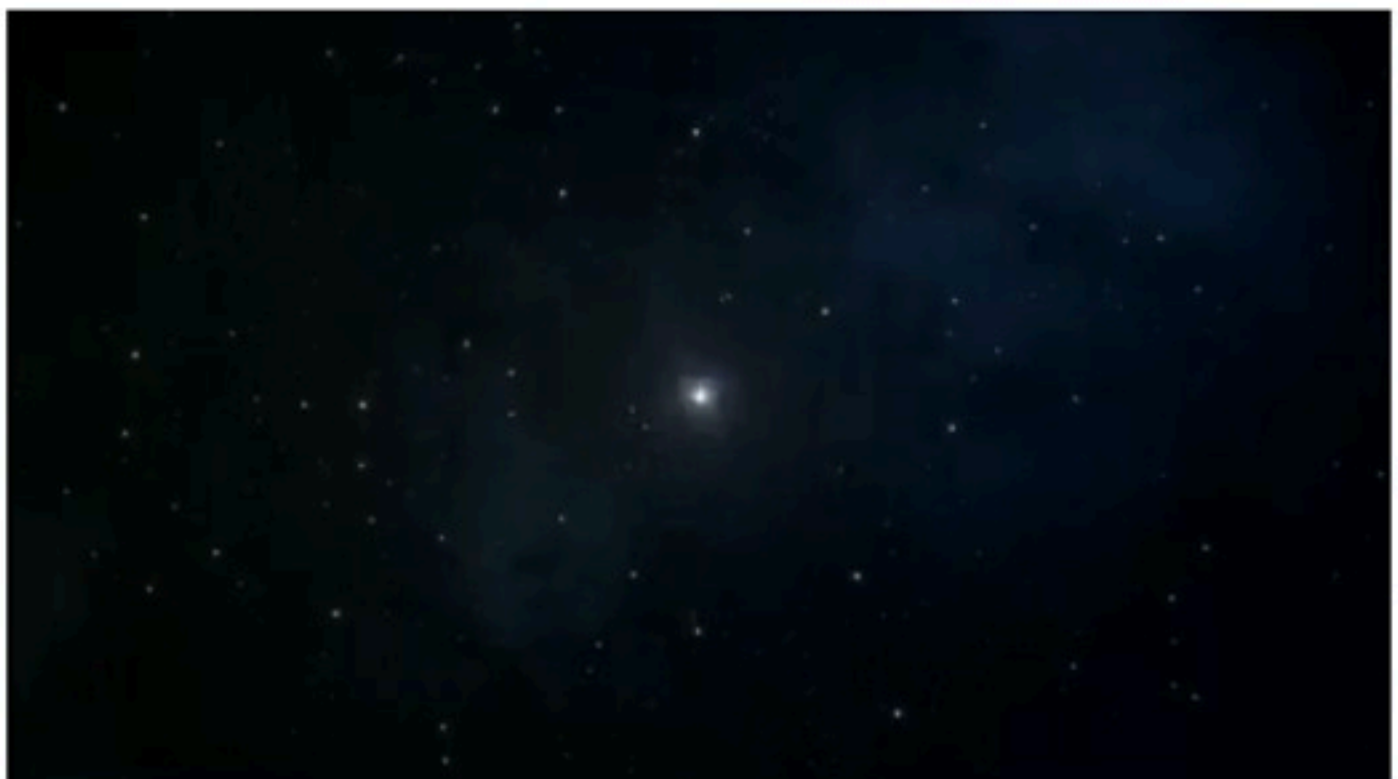

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Ancient monuments give us clues to astonishing past civilizations -- but they're under threat from pollution, war, neglect. Ben Kacyra, who invented a groundbreaking 3D scanning system, is using his invention to scan and preserve the world's heritage 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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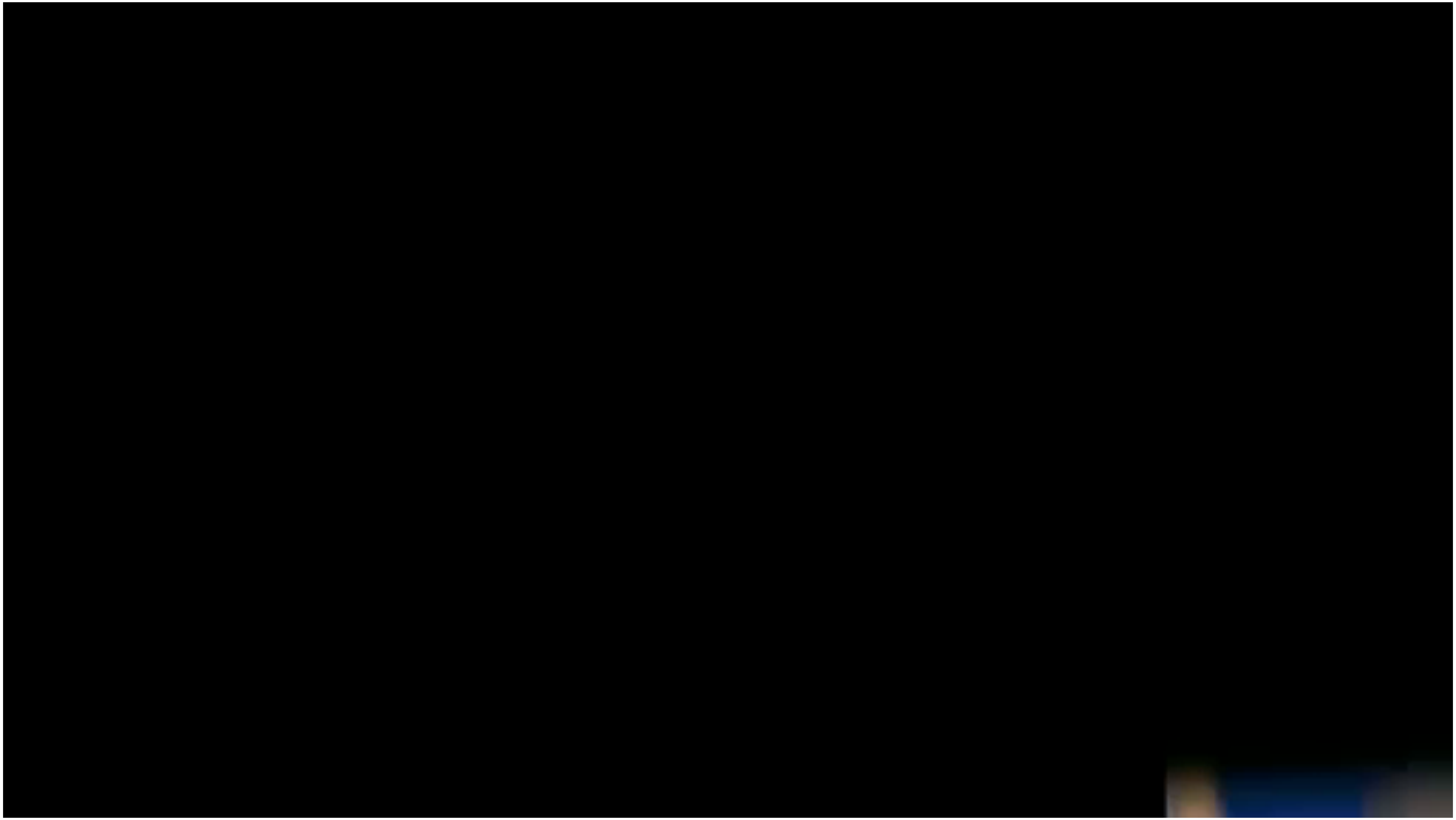

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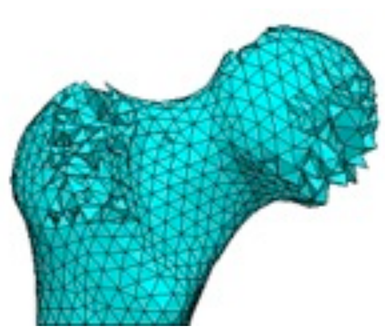
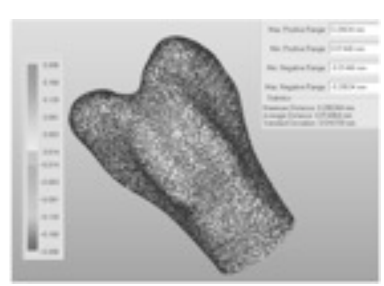
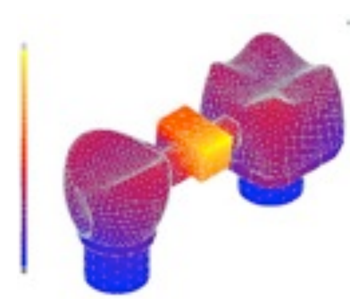
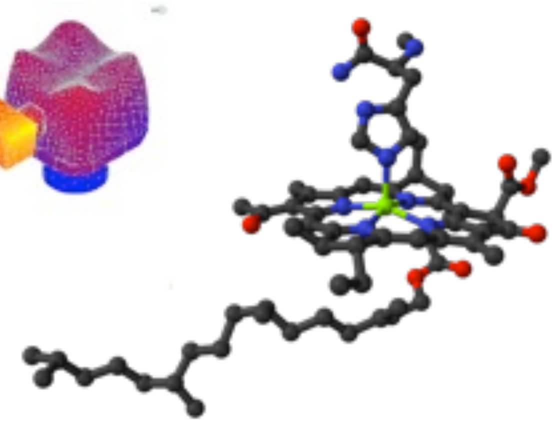


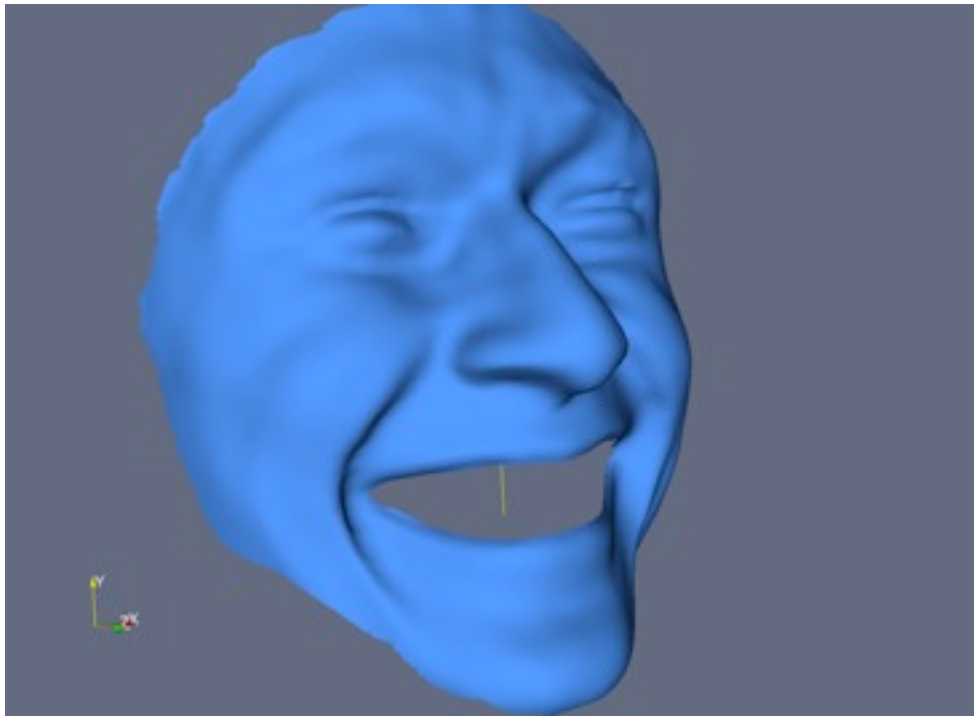

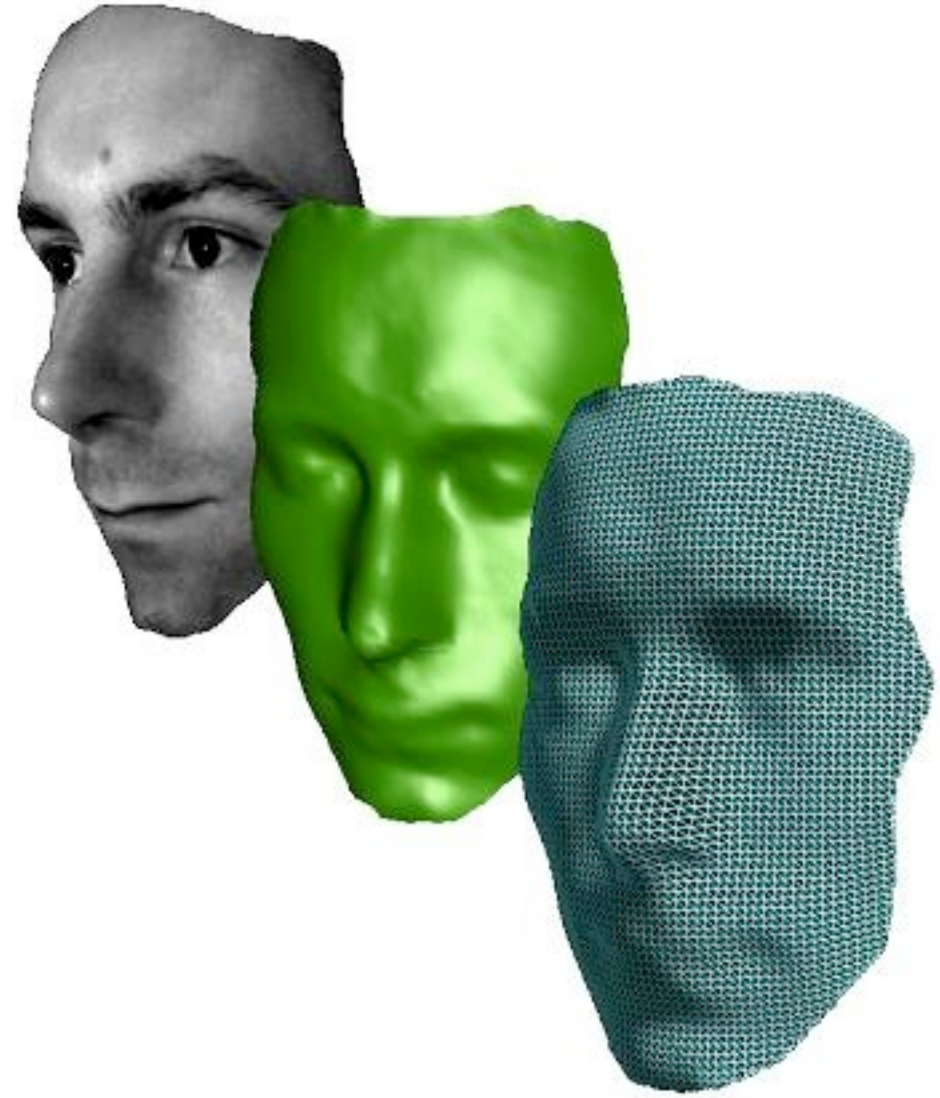

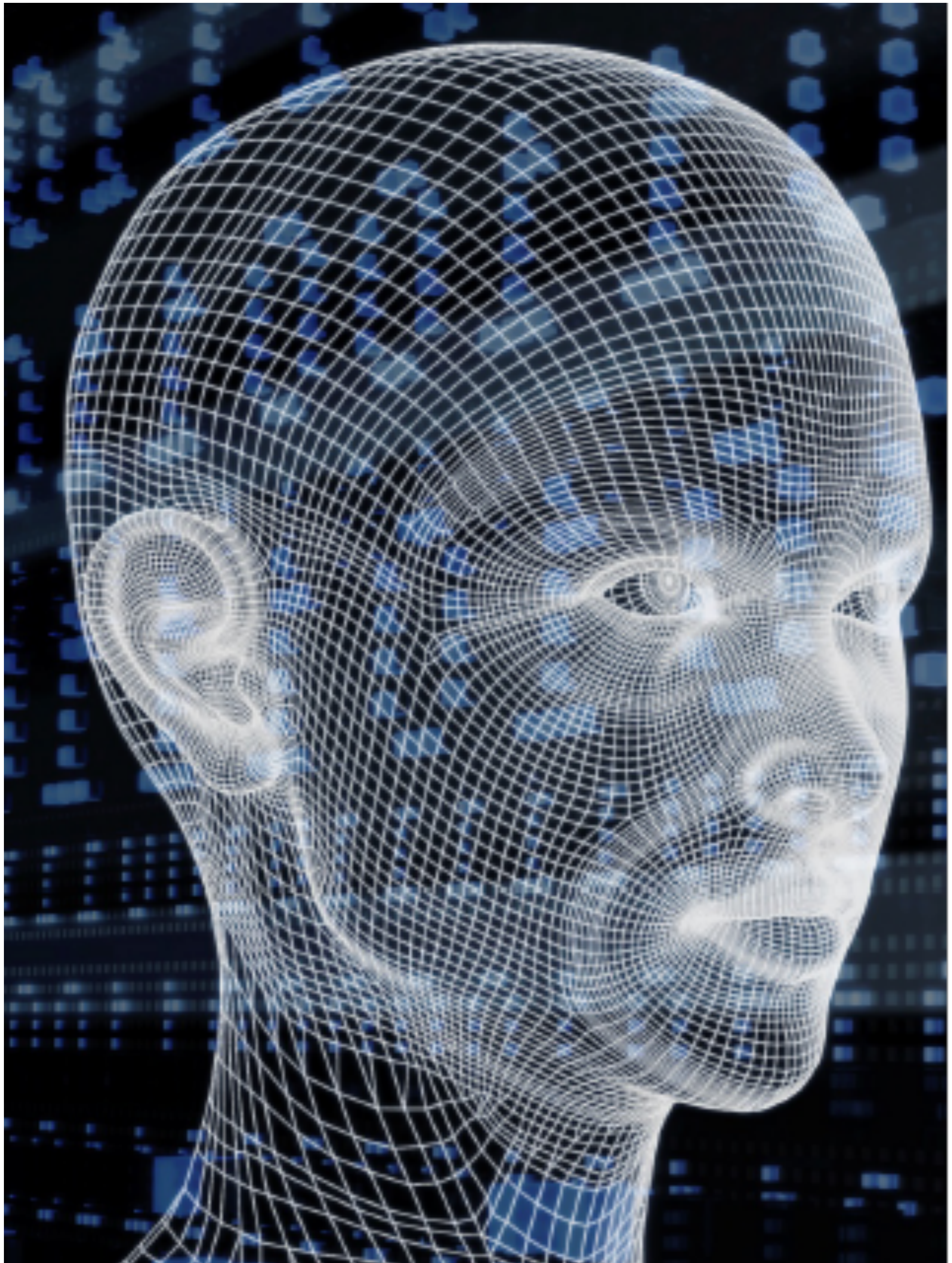

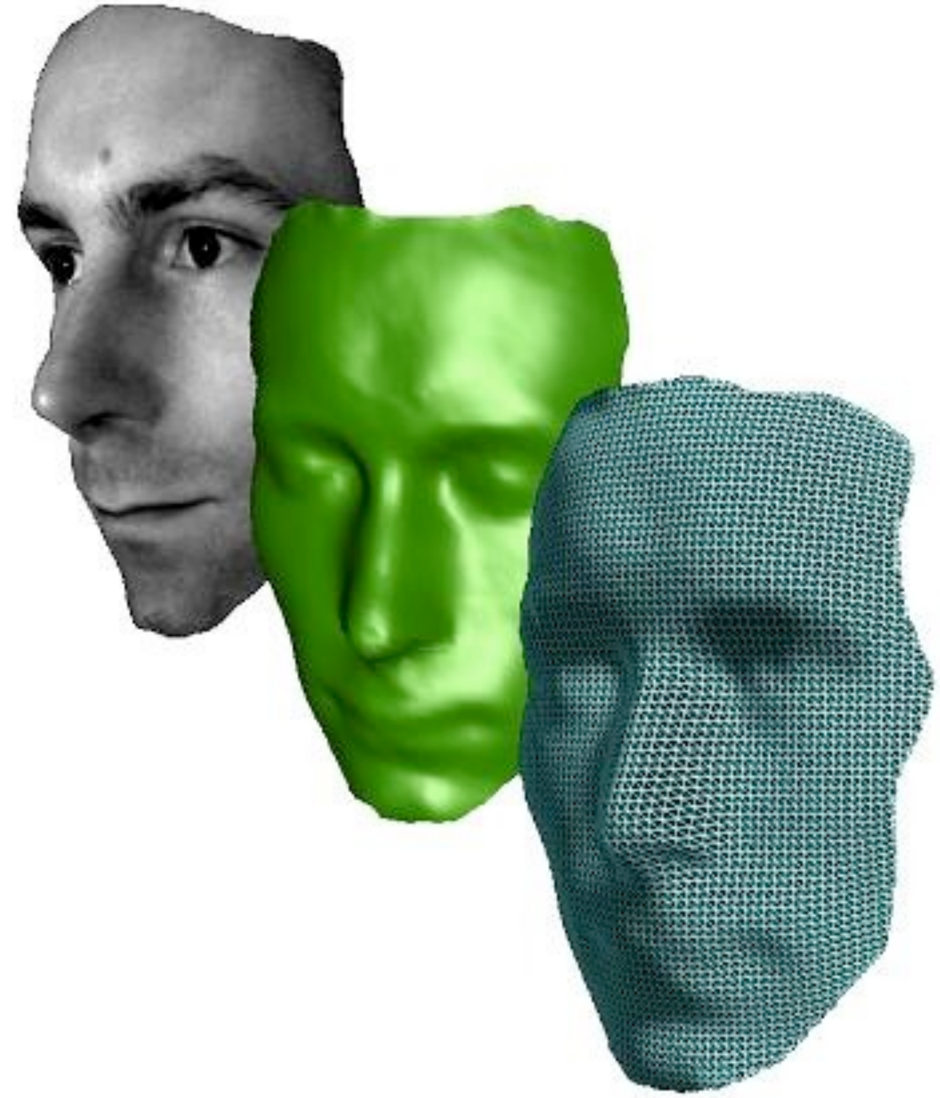


3D Face Biometrics 2013
Shangai, China - April 22, 2013
In conjunction with the 10th IEEE International Conference on Automatic Face and Gesture Recognition

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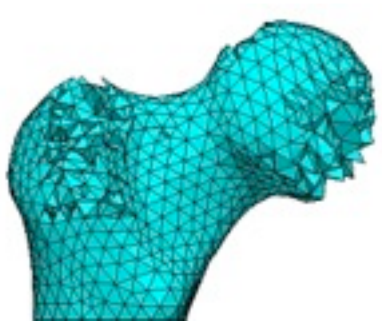
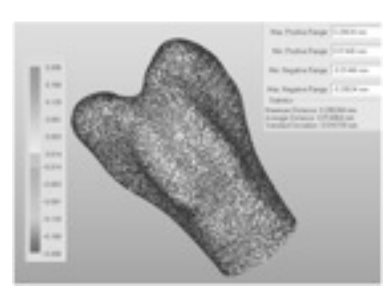
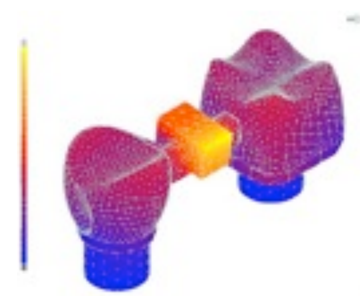
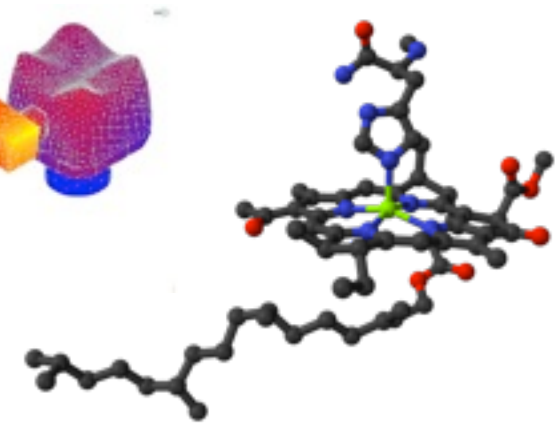
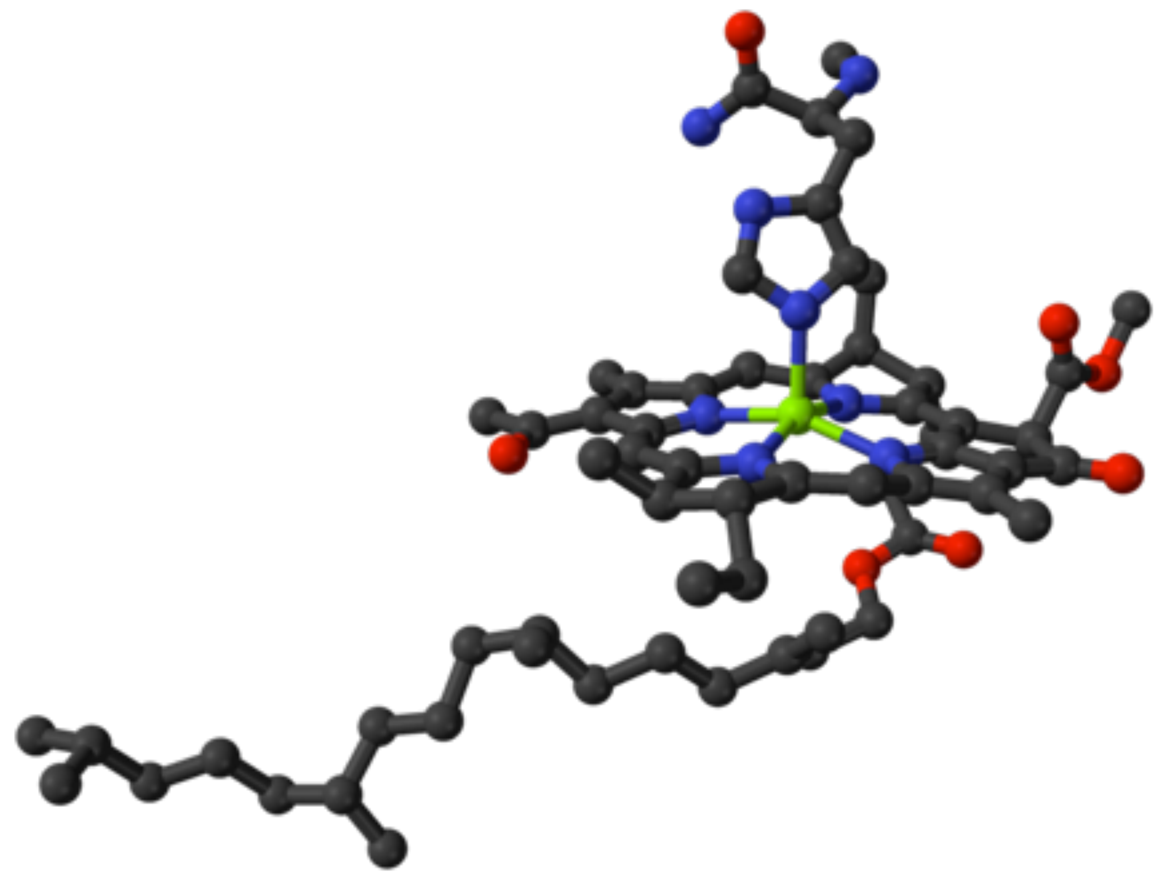
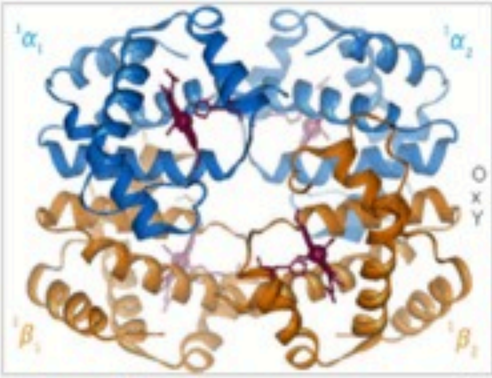





Structural biology

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."



Hemoglobin, the oxygen transporting protein found in red blood cells

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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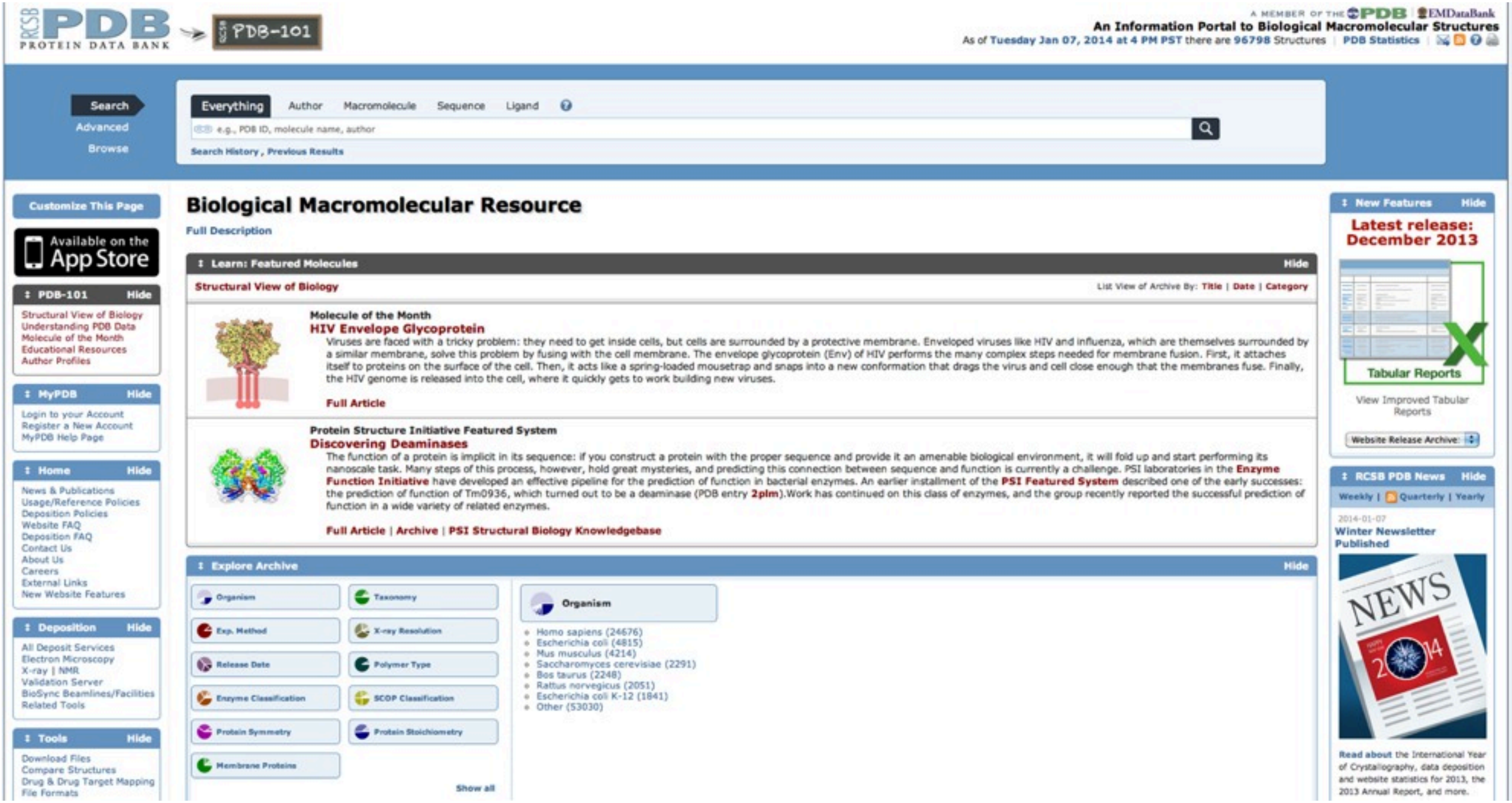
similarity principle:

geometrically similar molecules are likely to have similar functions



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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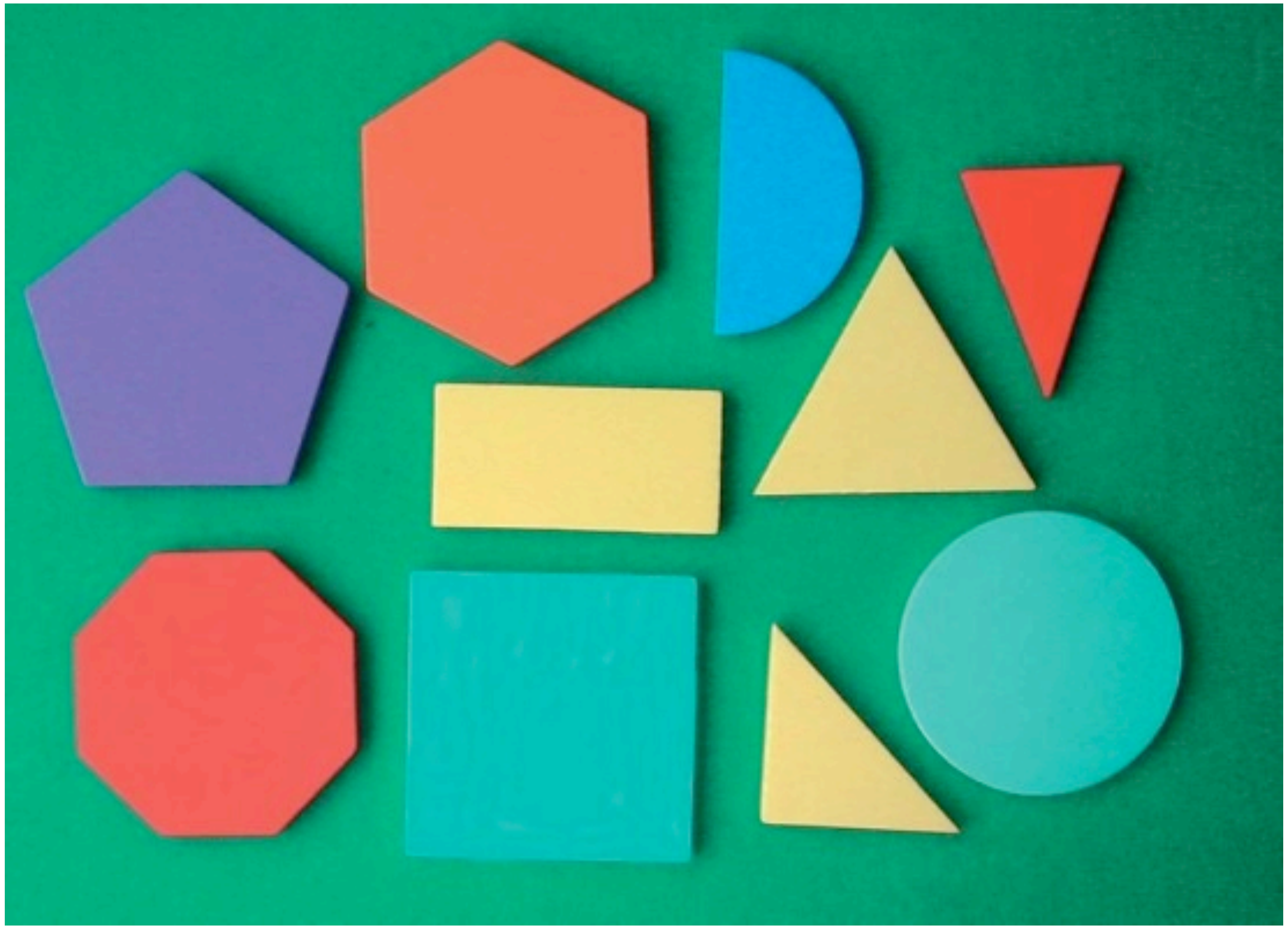
Cheminformatics

From Wikipedia, the free encyclopedia
(Redirected from Chemoinformatics)

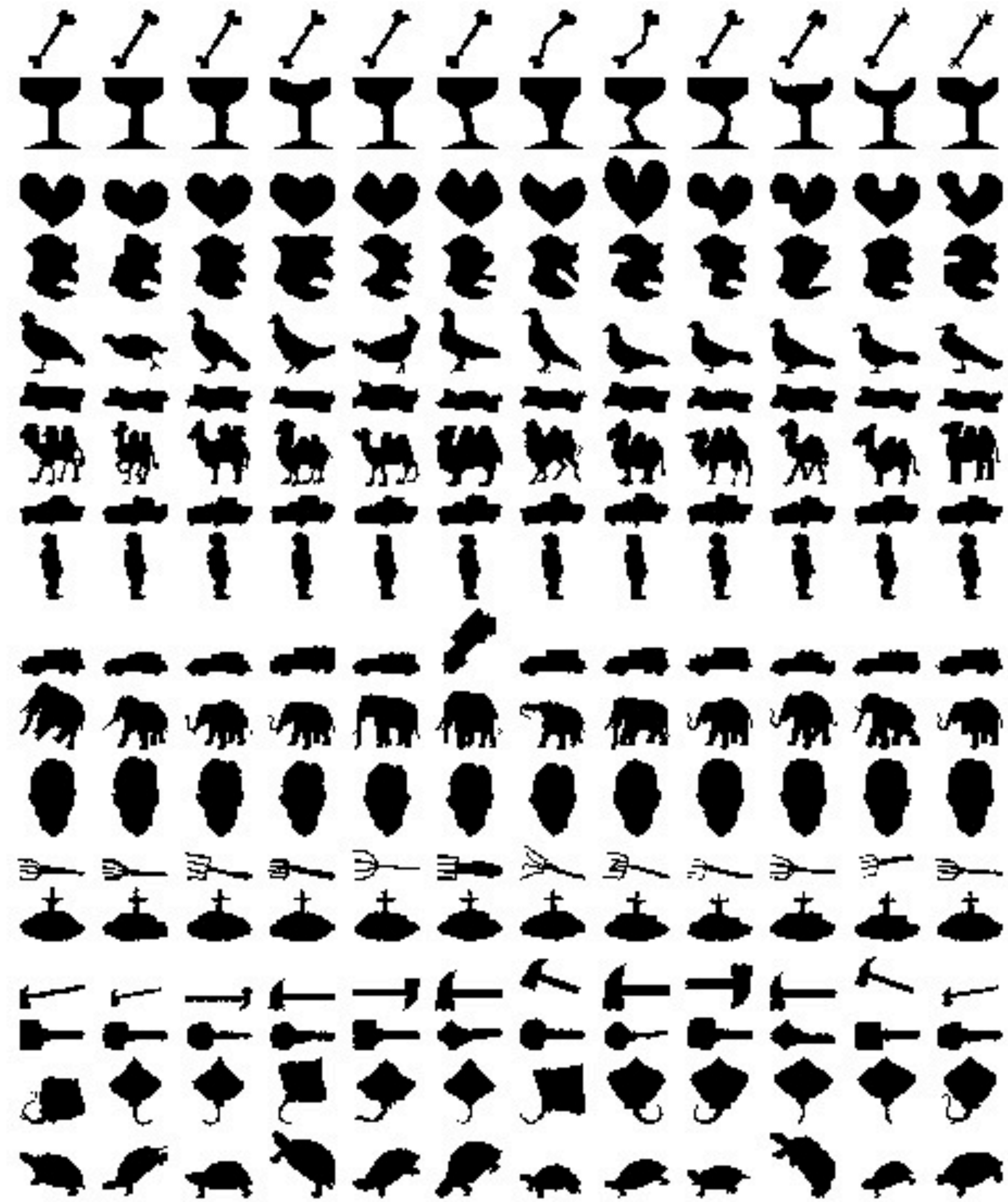
Cheminformatics (also known as **chemoinformatics, chemioinformatics** and **chemical informatics**) is the use of computer and informational techniques applied to a range of problems in the field of chemistry. These *in silico* techniques are used in, for example, pharmaceutical companies in the process 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

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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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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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Data for MATLAB hackers

Here are some datasets in MATLAB format. I'm working on better documentation, but if you decide to use one of these and don't have enough info, send me a note and I'll try to help. Also, if you discover something, let me know and I'll try to include it for others. There is a Matlab Tutorial here.

Handwritten Digits

- MNIST Handwritten Digits [data/mnist_all.mat]
  [training pictures: 0 1 2 3 4 5 6 7 8 9]
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  8-bit grayscale images of "0" through "9"; about 6K training examples of each class; 1K test examples
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  From Simon Lucas' (sml@essex.ac.uk), Algoval system.

Faces

- If you want a real face dataset, I strongly recommend the UMass project: Labelled Faces in the Wild.
- Frey Face [data/frey_rawface.mat] [picture]
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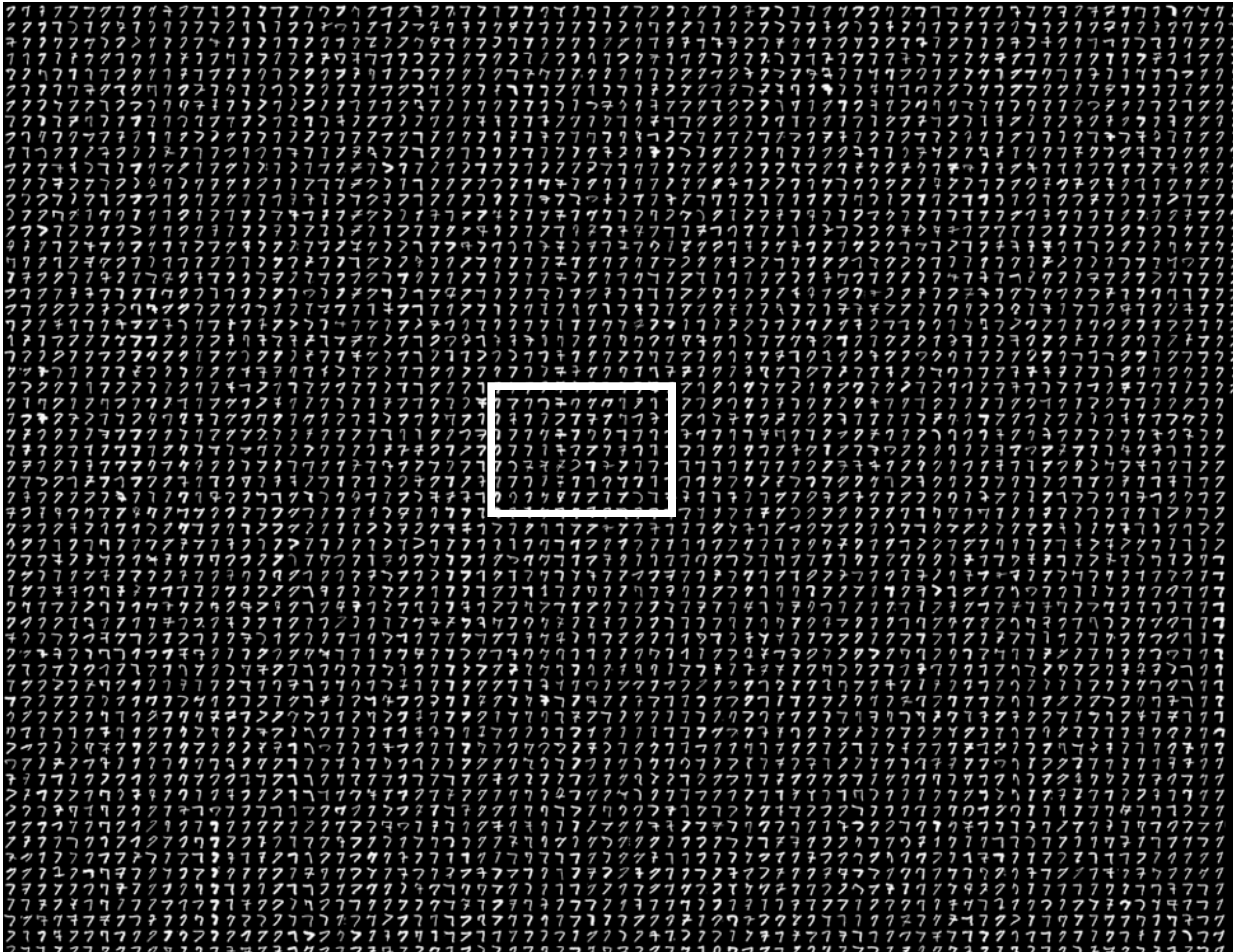
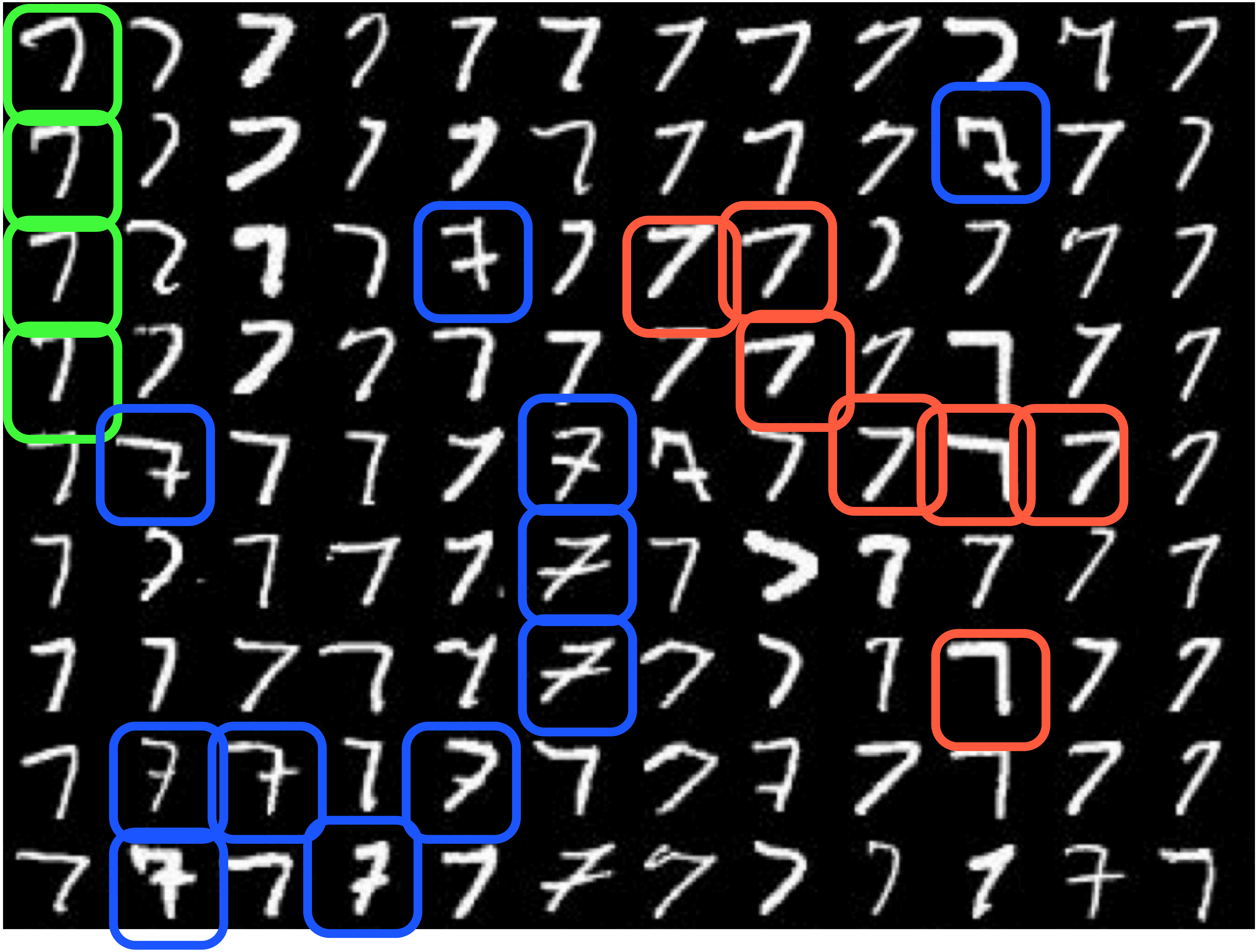
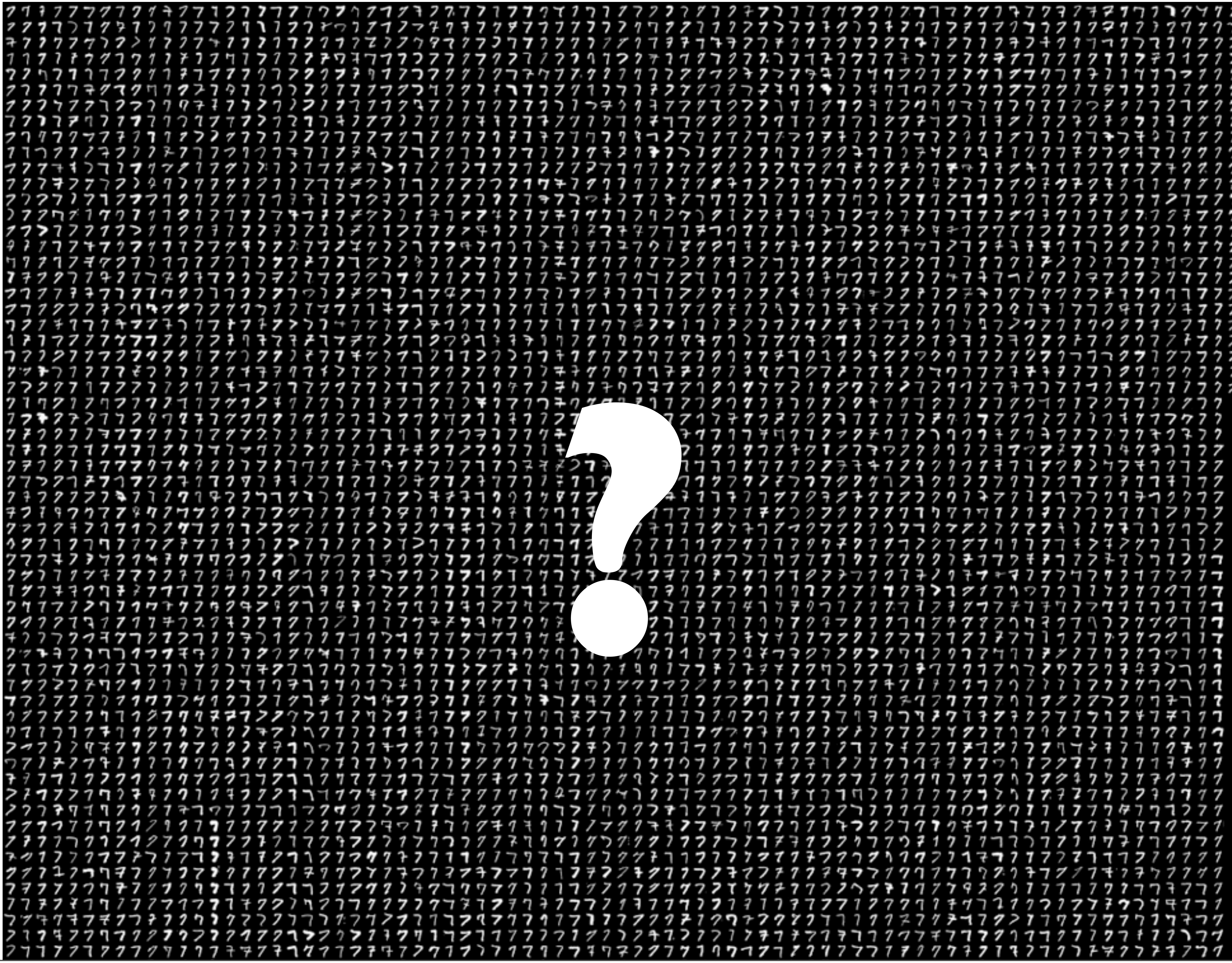


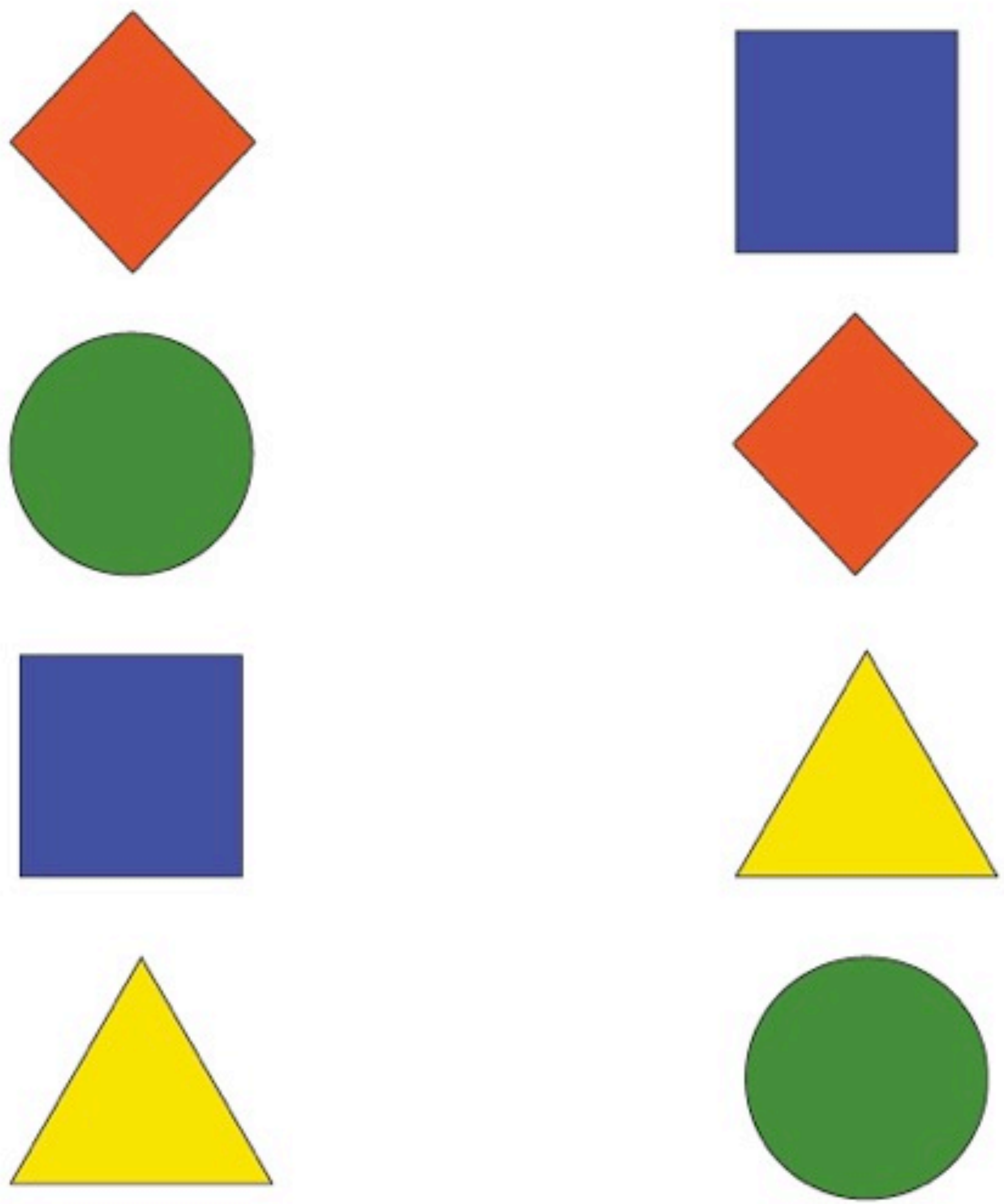




Name ______________________

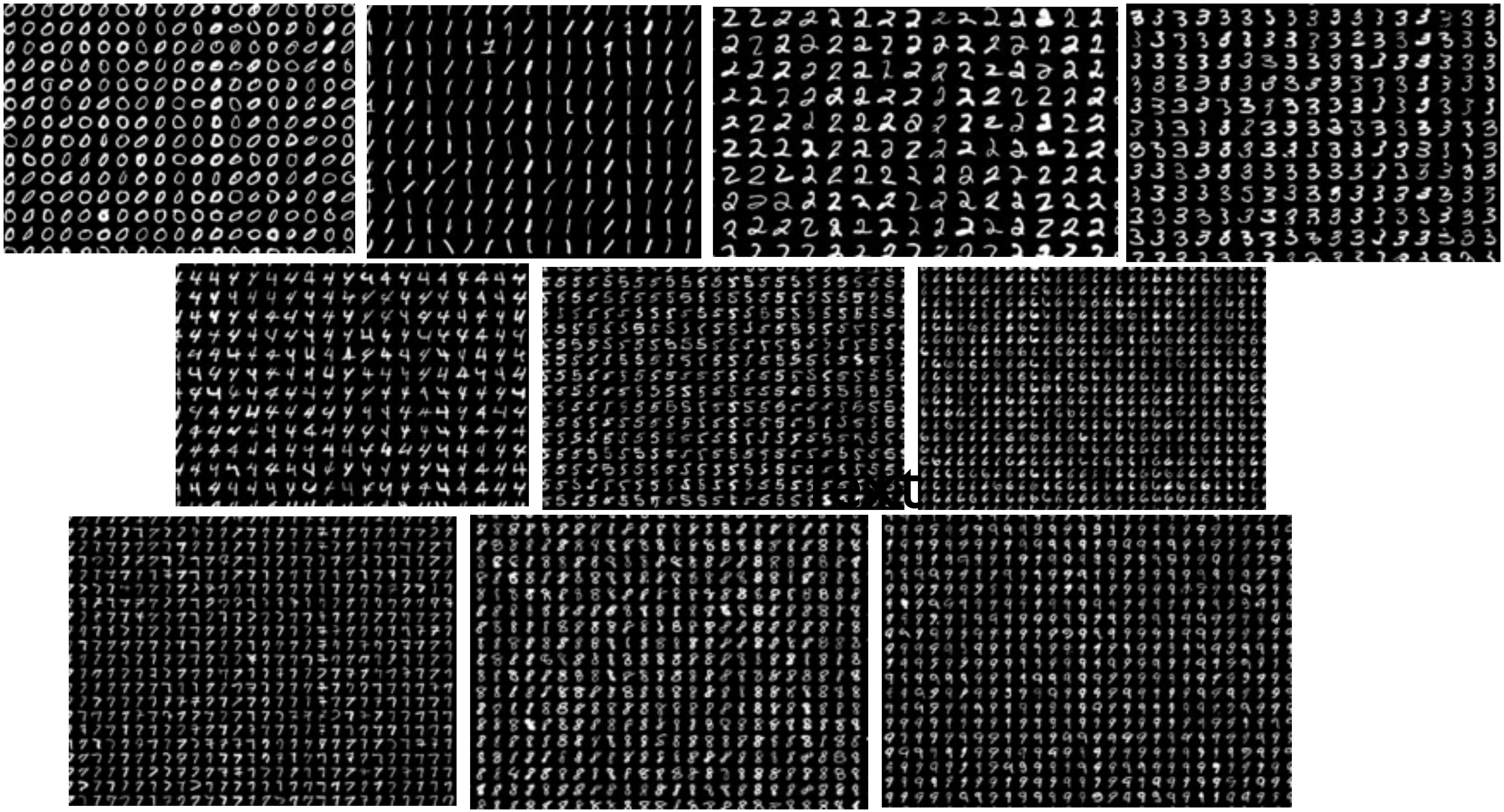
Shape Matching Worksheet

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



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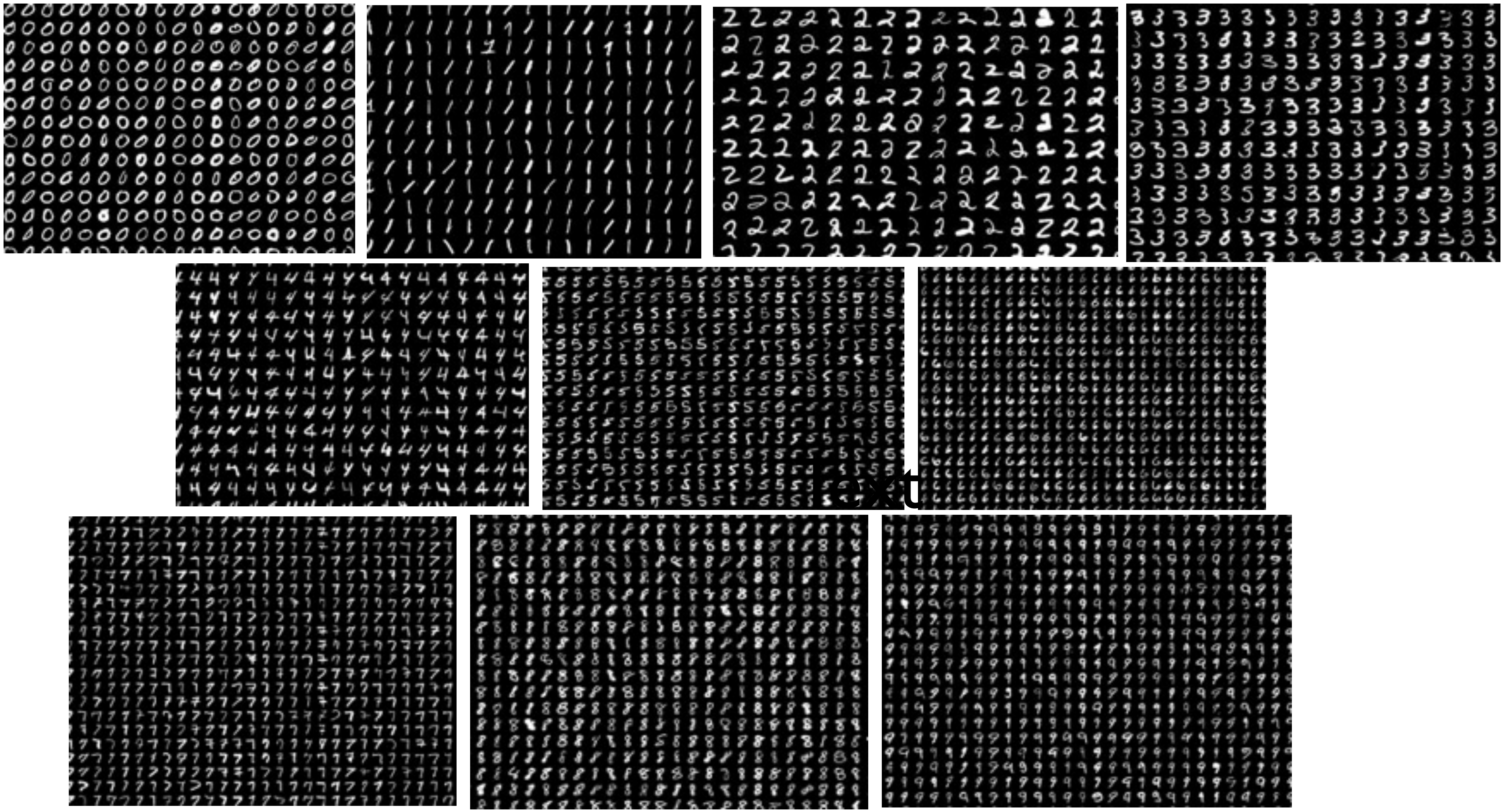
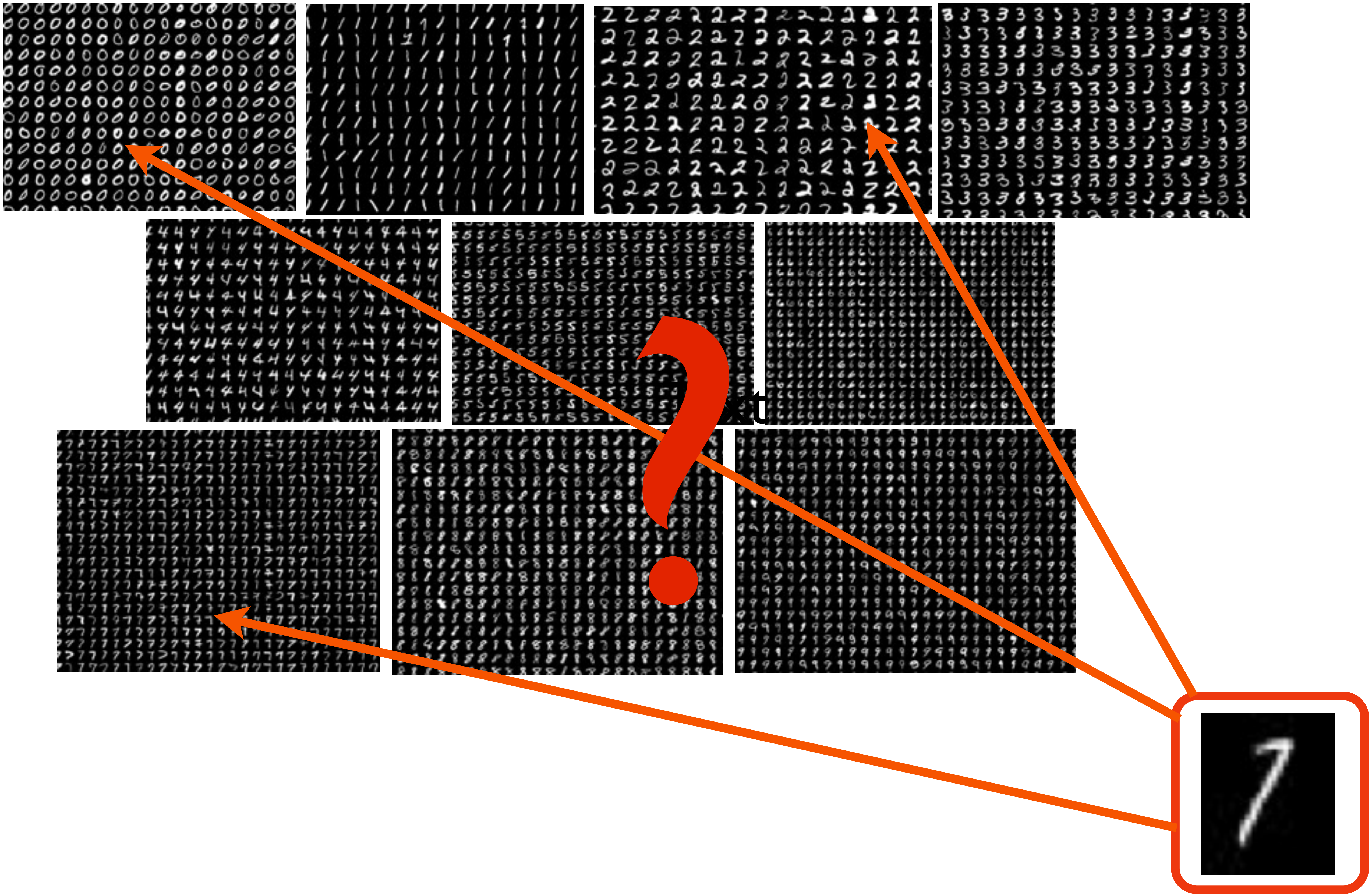


typical scenario



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 $\mathcal{D}$:

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

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

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

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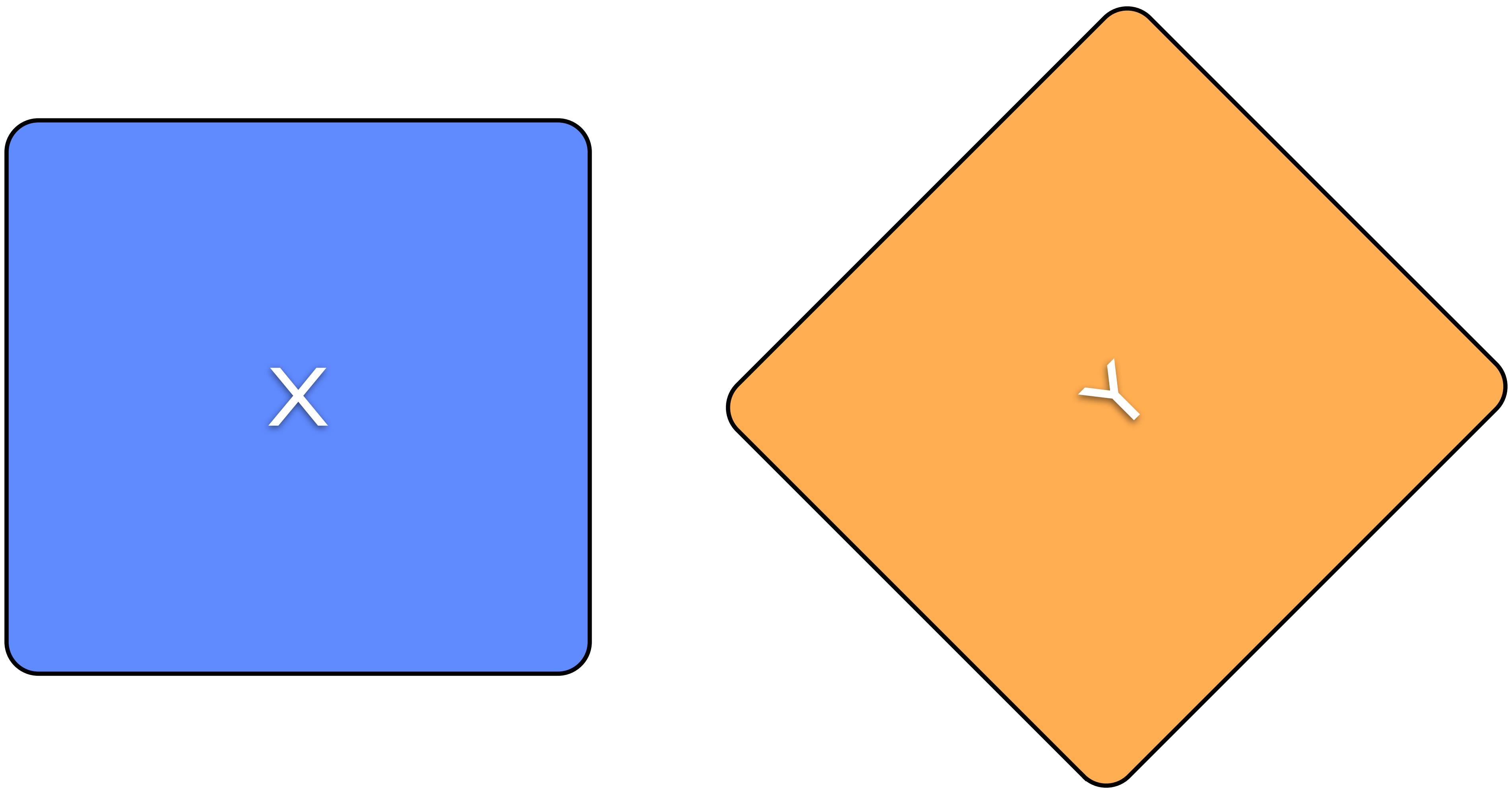
- in order to do this, one first needs to define a notion **dist** of *distance* or *dis-similarity between objects*.

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?



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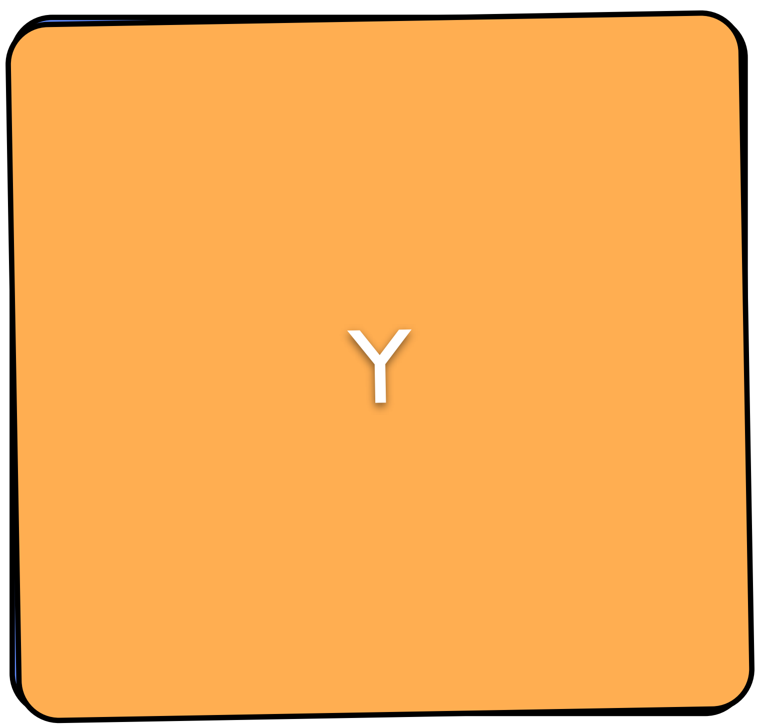
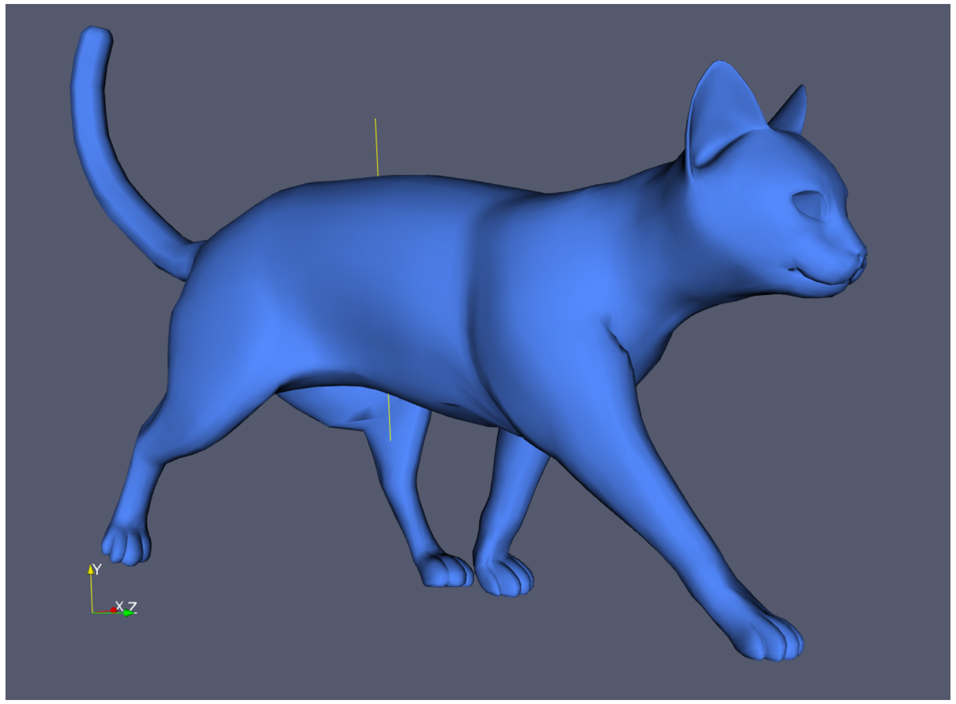
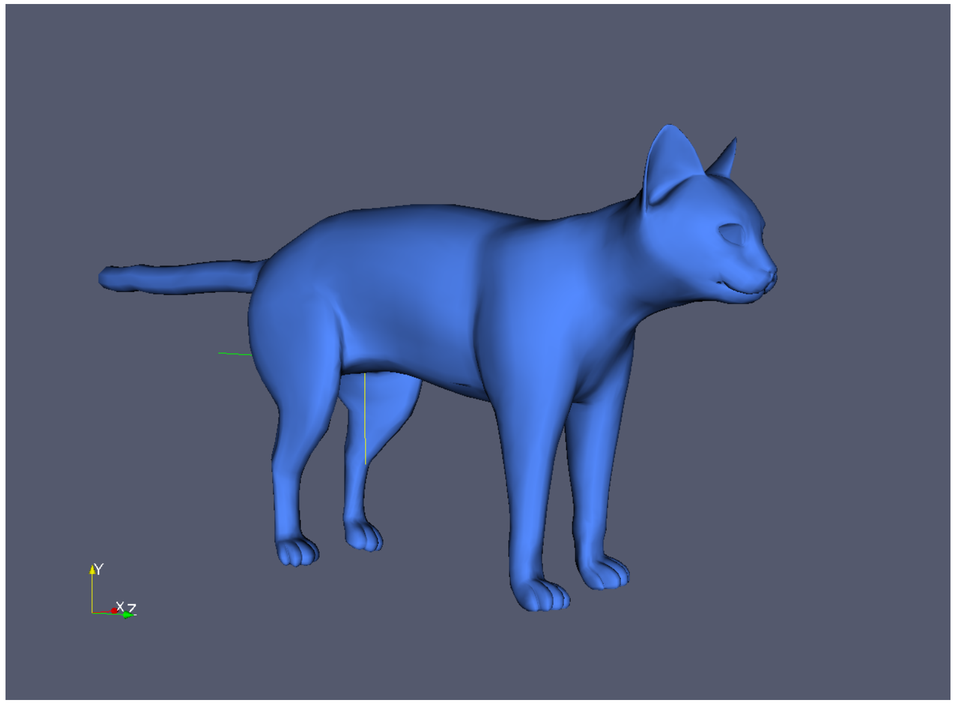


this is called invariance to *rigid transformations*

Another important points: invariances

what about these two?

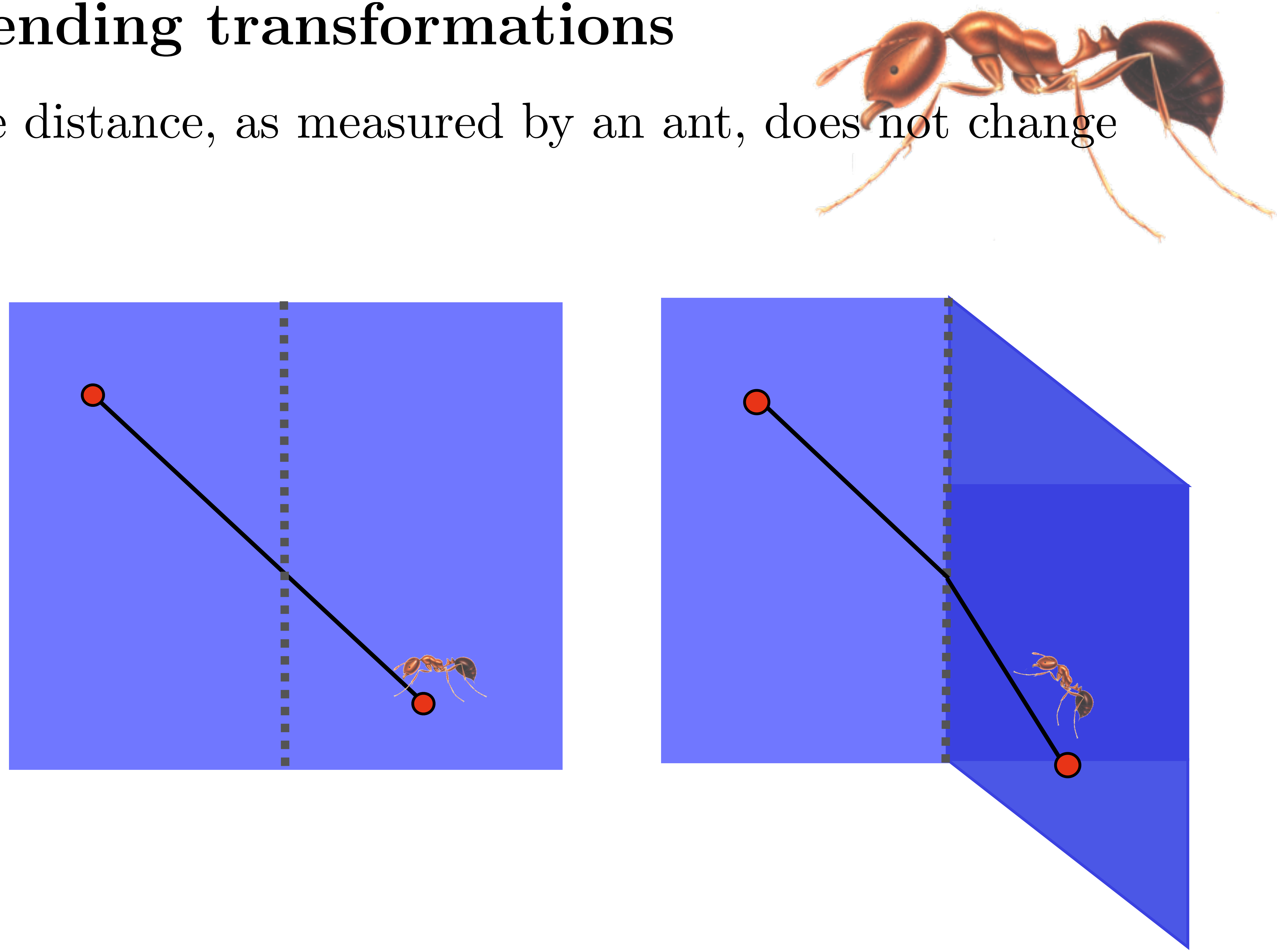




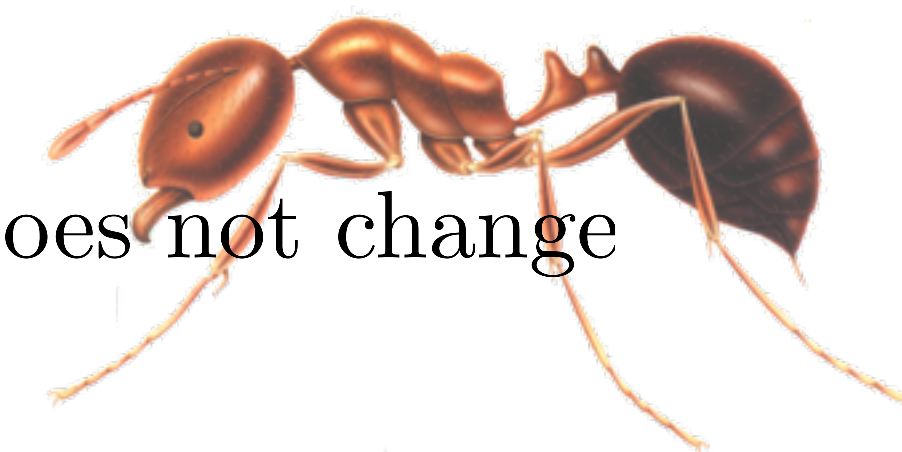
roughly speaking, this corresponds to invariance to *bending transformations*..

Bending transformations

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



Bending transformations



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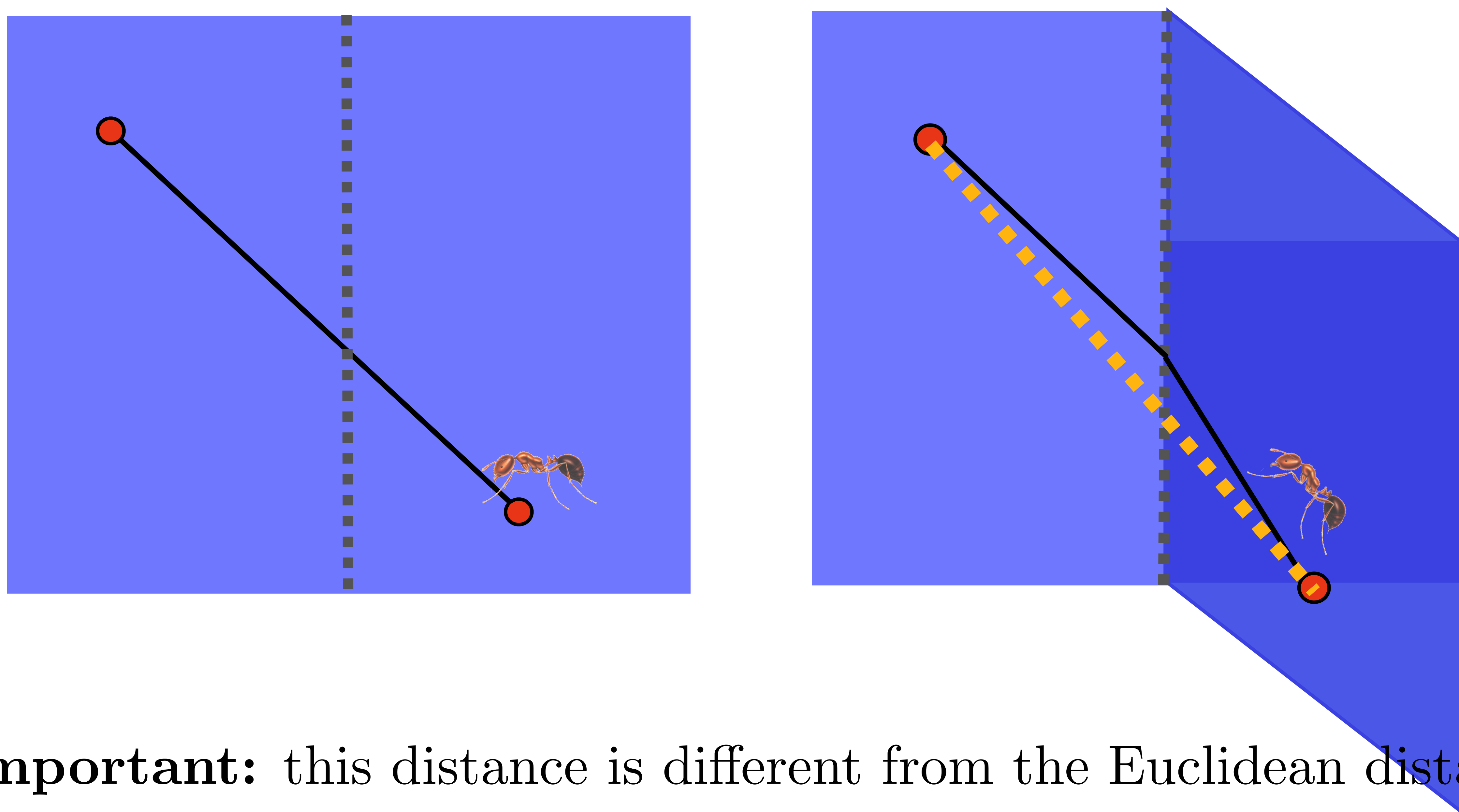
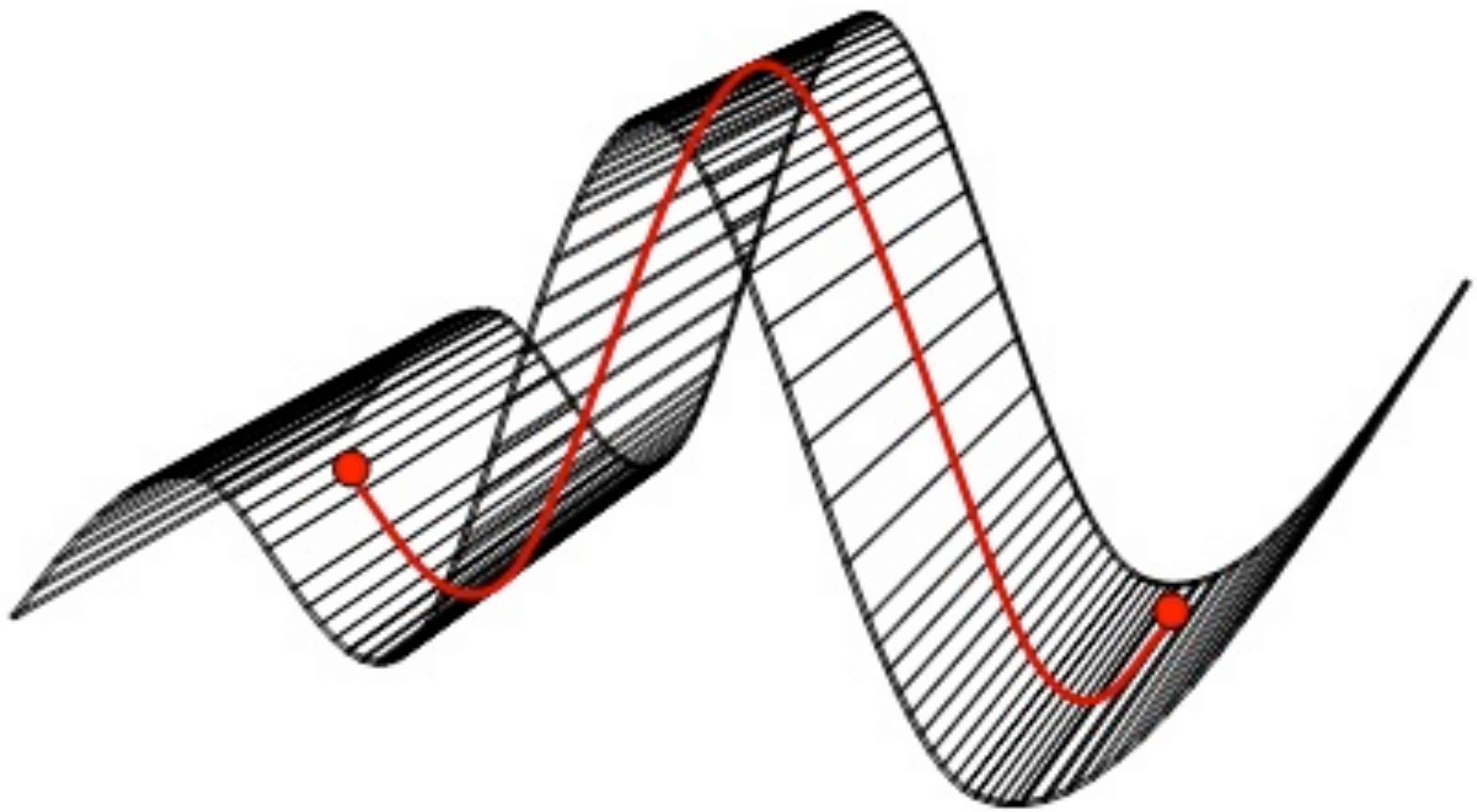
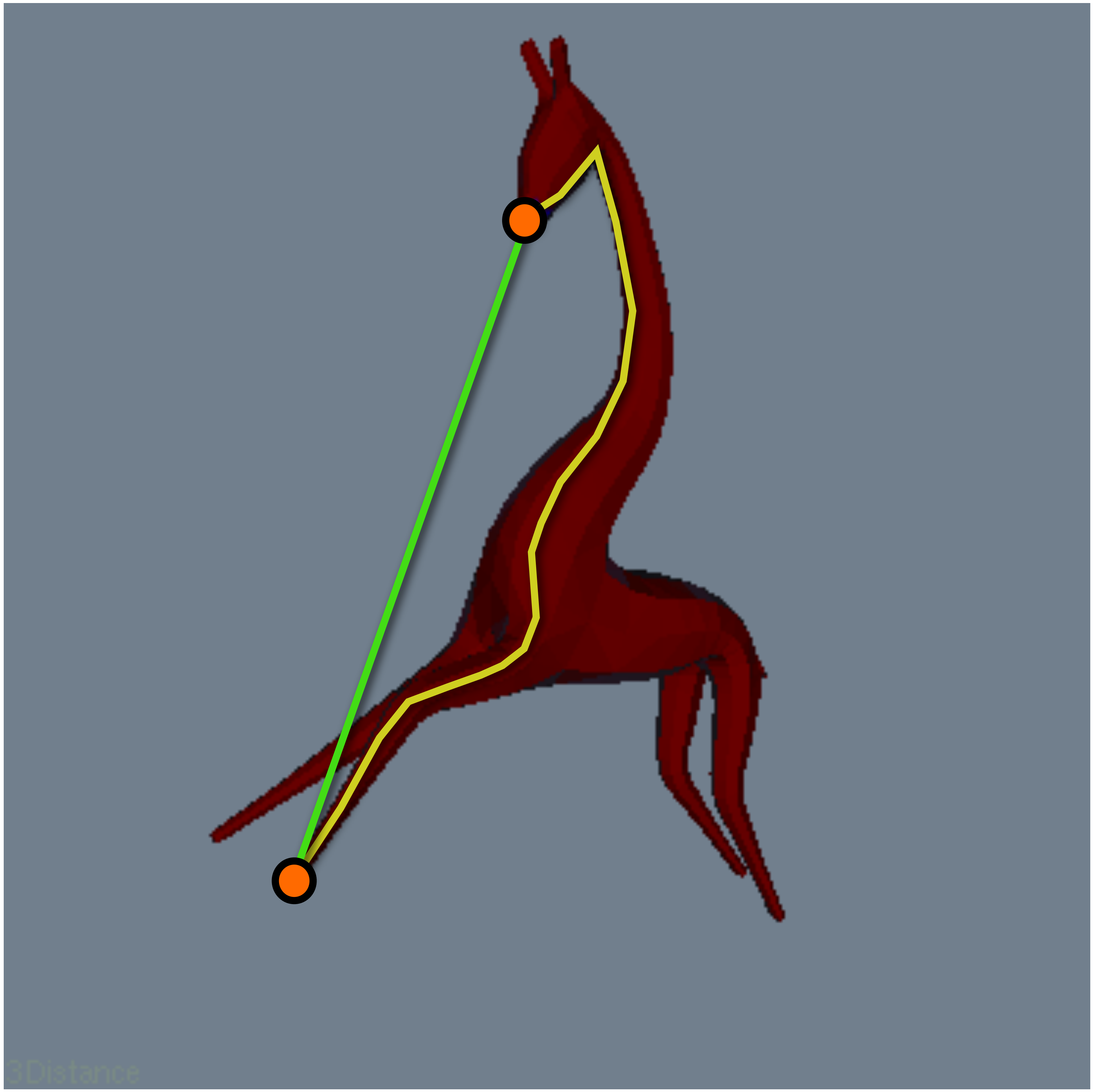


Important: this distance is different from the Euclidean distance!!



Geodesic distance vs Euclidean distance



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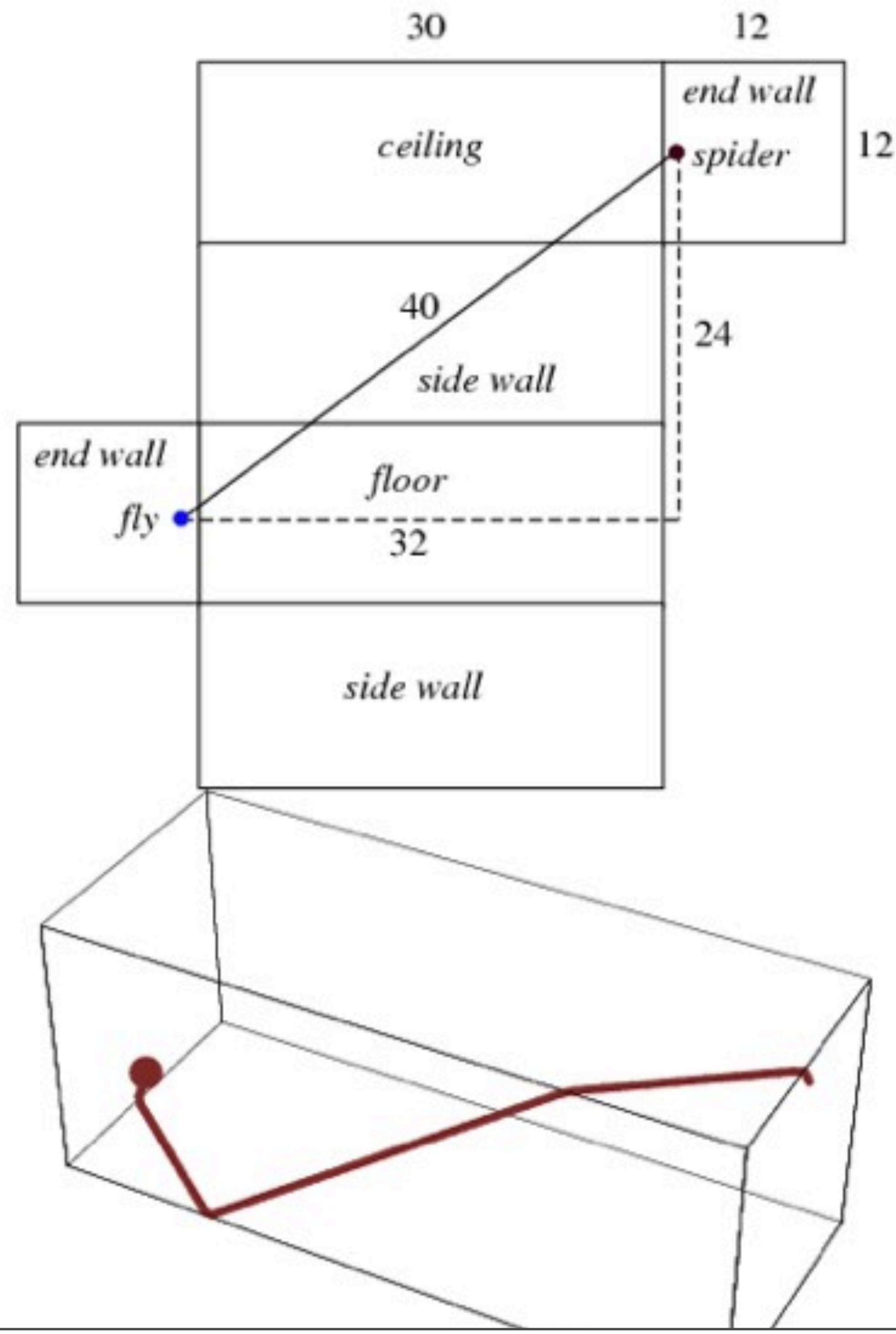
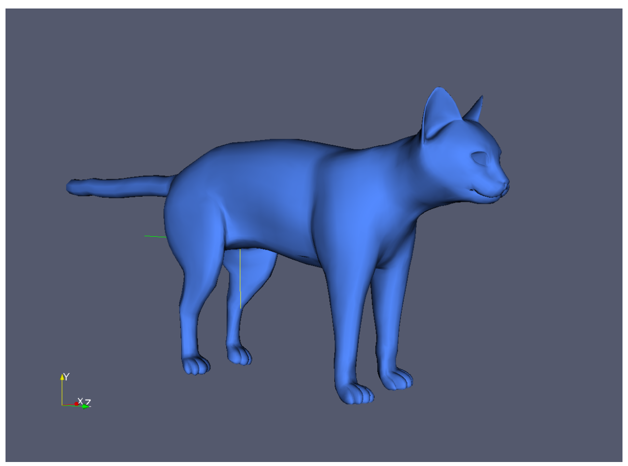
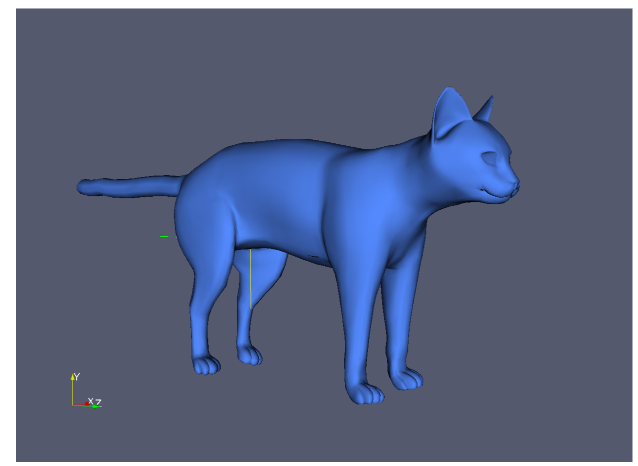
Spider and Fly Problem

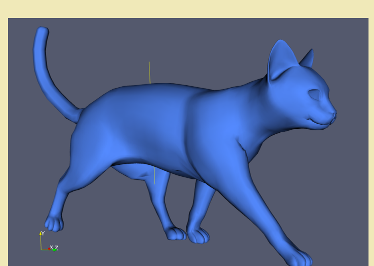
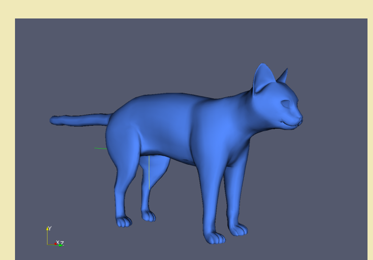
DOWNLOAD *Mathematica* Notebook



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 $d : X \times X \to \mathbb{R}^+$, called the metric, s.t.

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

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

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!