Tutorial 3
Comparing Biological Shapes

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What is a shape?

A shape is a 2-manifold with a **Riemannian metric** (angle, distance, surface area, volume, derivatives,…)

Discrete representations of shapes

1) **Continuous surfaces**
    1) Manifolds
    2) Metric on manifolds
    3) Topology
    4) Orientation

2) **Sets of points and triangulations**
    1) Simplicial complexes
    2) Triangulations
    3) Delaunay and applications

3) **Discrete Surfaces**
    1) Meshes
    2) Manifold/ orientation
    3) Geometry / topology

4) **Manipulating discrete surfaces**
    1) Basic mesh operations
    2) Remeshing

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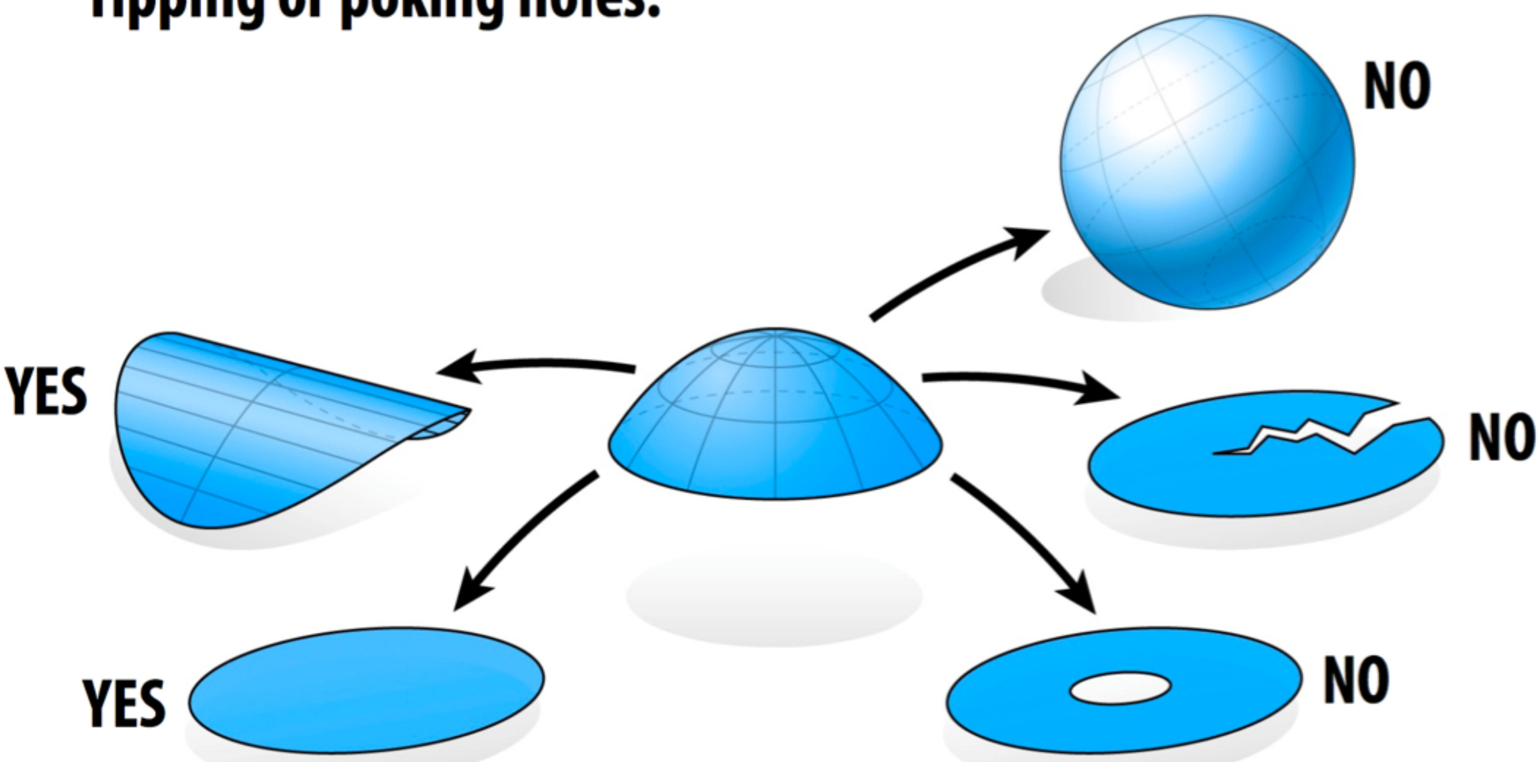
What is a manifold?

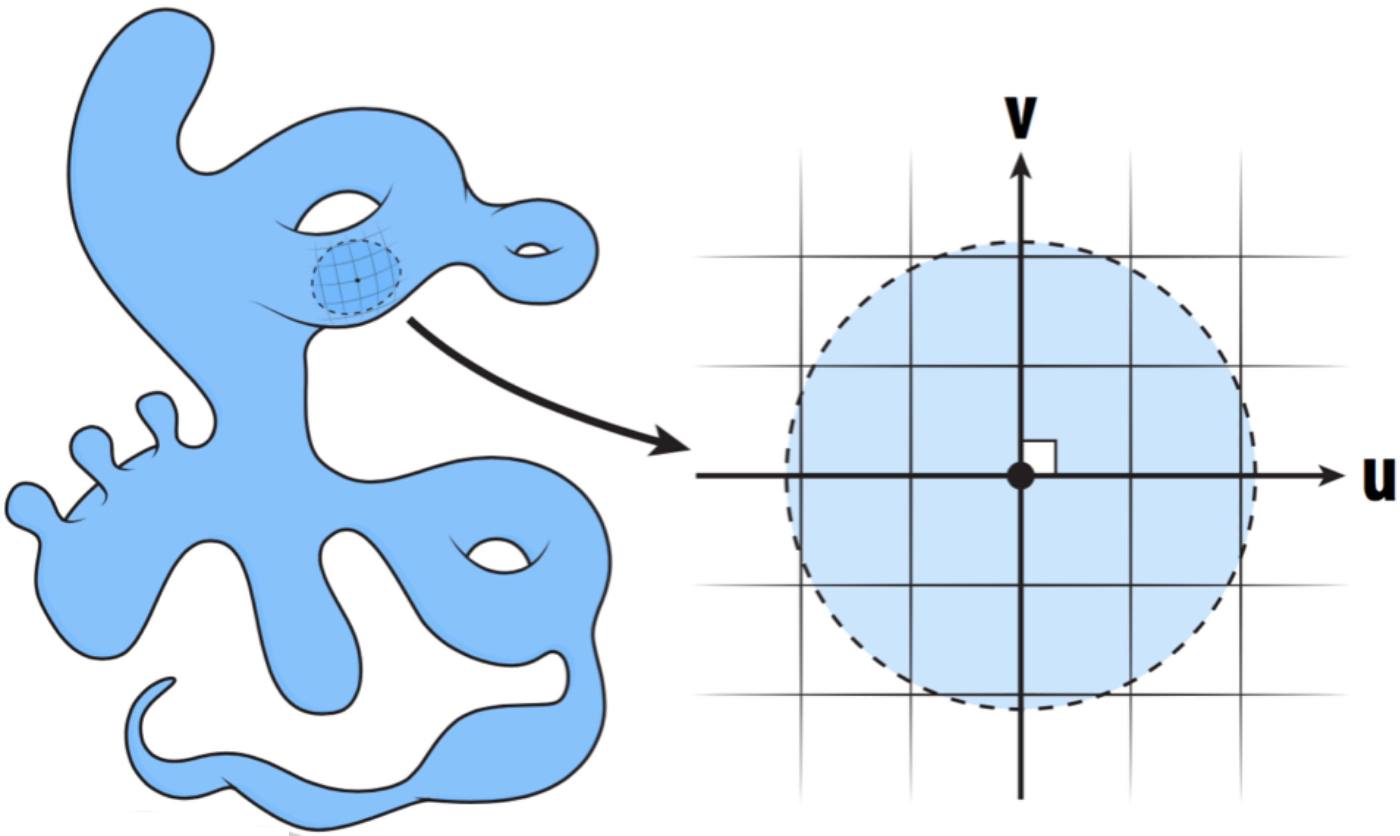
"A subset S of R^m is an n-manifold if every point p in S is contained in a neighborhood that can be mapped bijectively and continuously (both ways) to the open ball in R^n."

In other words: each little piece can be made flat without "ripping or poking holes."

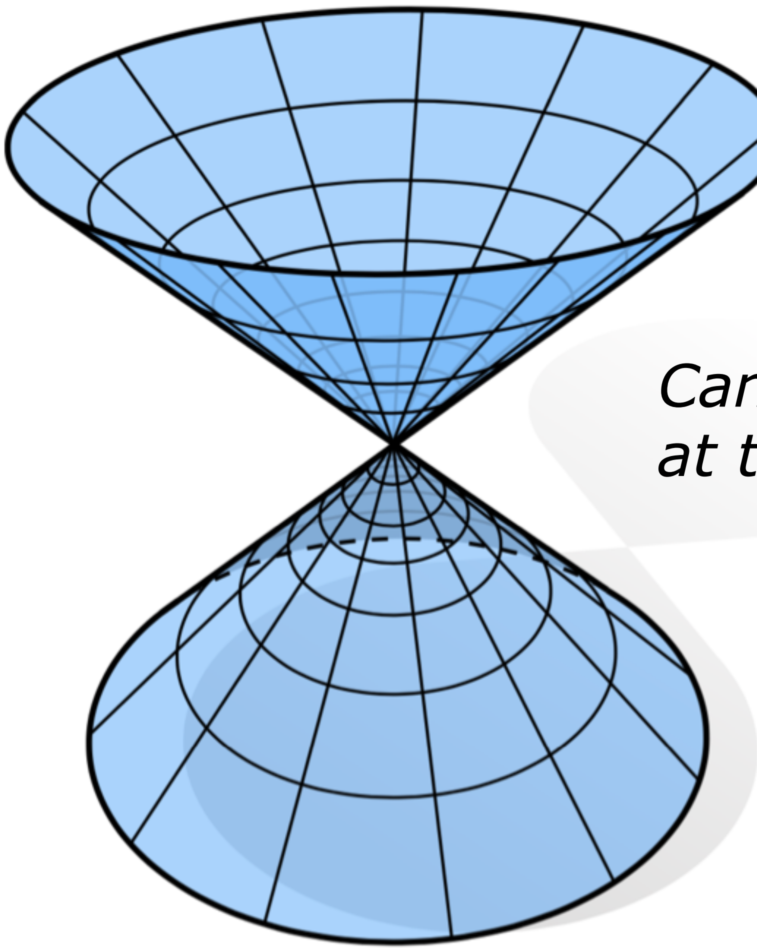


Why a manifold?

- All surfaces look similar (at least locally)
- We can set a (local) coordinate system



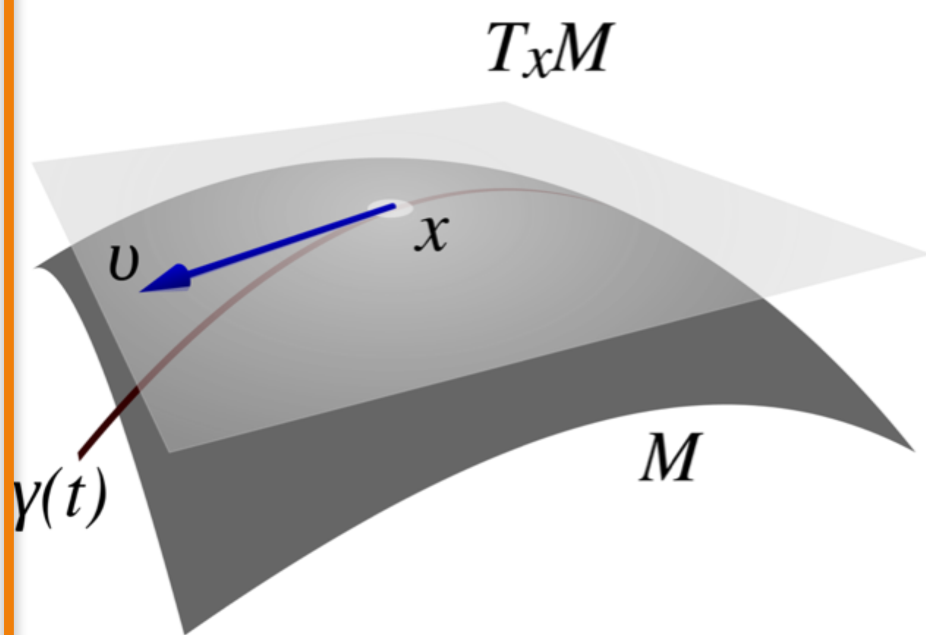
Not every surface is a manifold



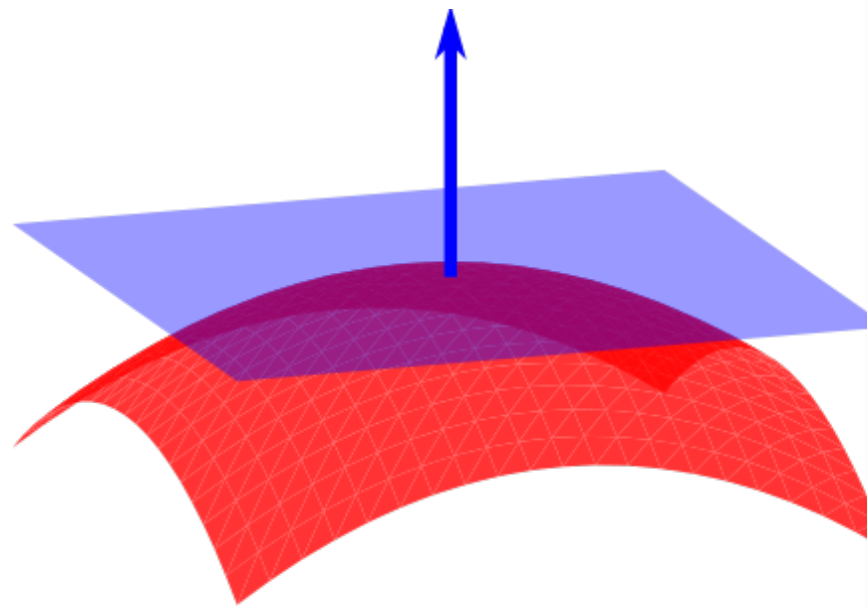
Cannot set a coordinate system at the junction point…

Riemannian Manifold

Tangent space:



Normal:

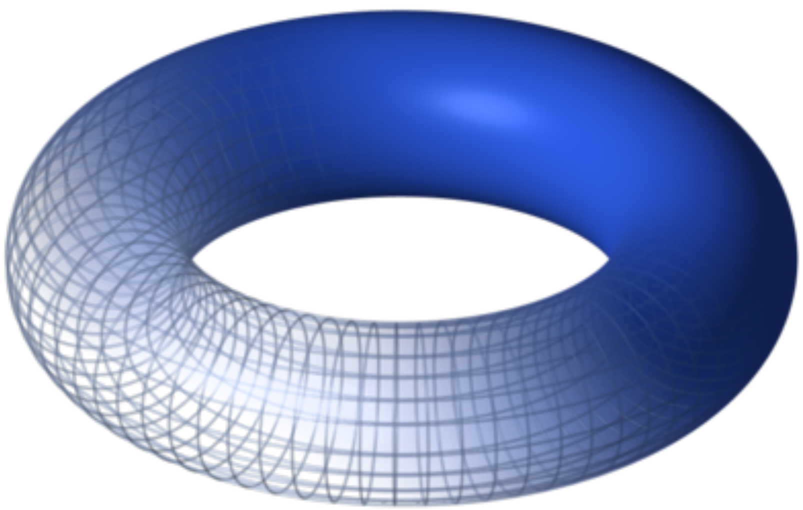


Metric tensor:

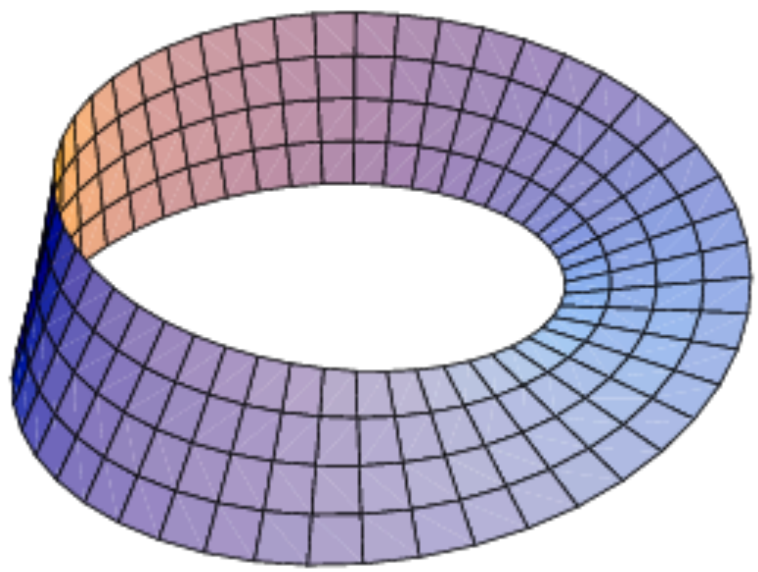
$$g: \quad (T_xM, T_xM) \rightarrow R$$
$$(u,v) \qquad \rightarrow g(u,v)$$

Orientation of a manifold

Orientability of a surface: a property of surfaces in Euclidean space that measures whether it is possible to make a consistent choice of surface normal vector at every point.

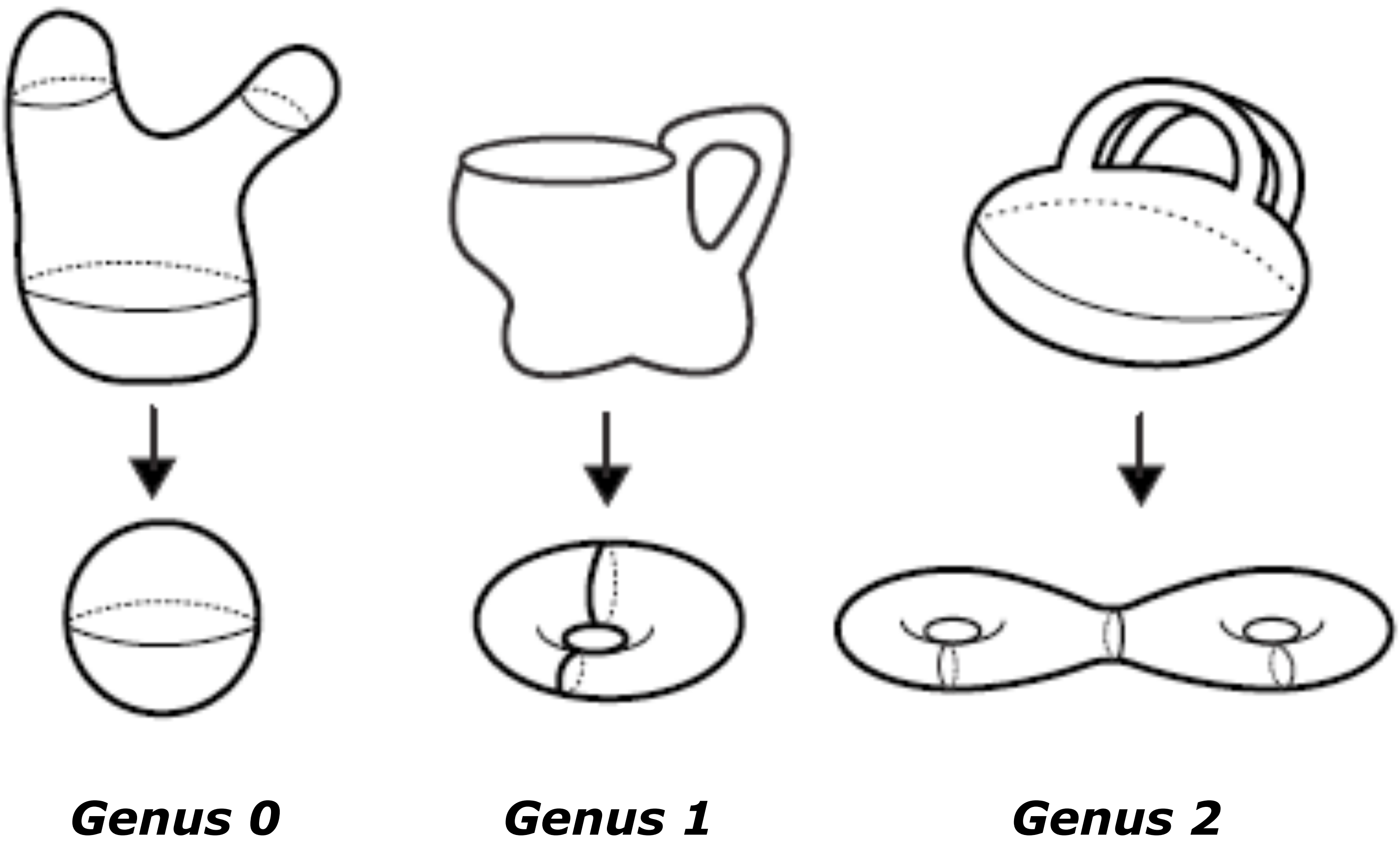


Orientable



Non orientable

Topology of a surface



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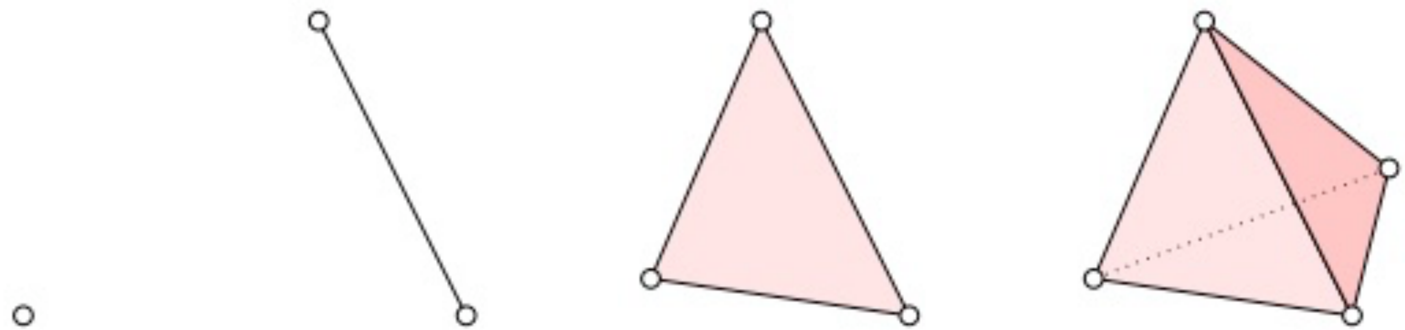
Simplices

Definition: A ***k-simplex*** is a k-dimensional polytope which is the convex hull of its k+1 vertices



0-simplex (vertex) | 1-simplex (edge) | 2-simplex (triangle) | 3-simplex (tetrahedron) | .....

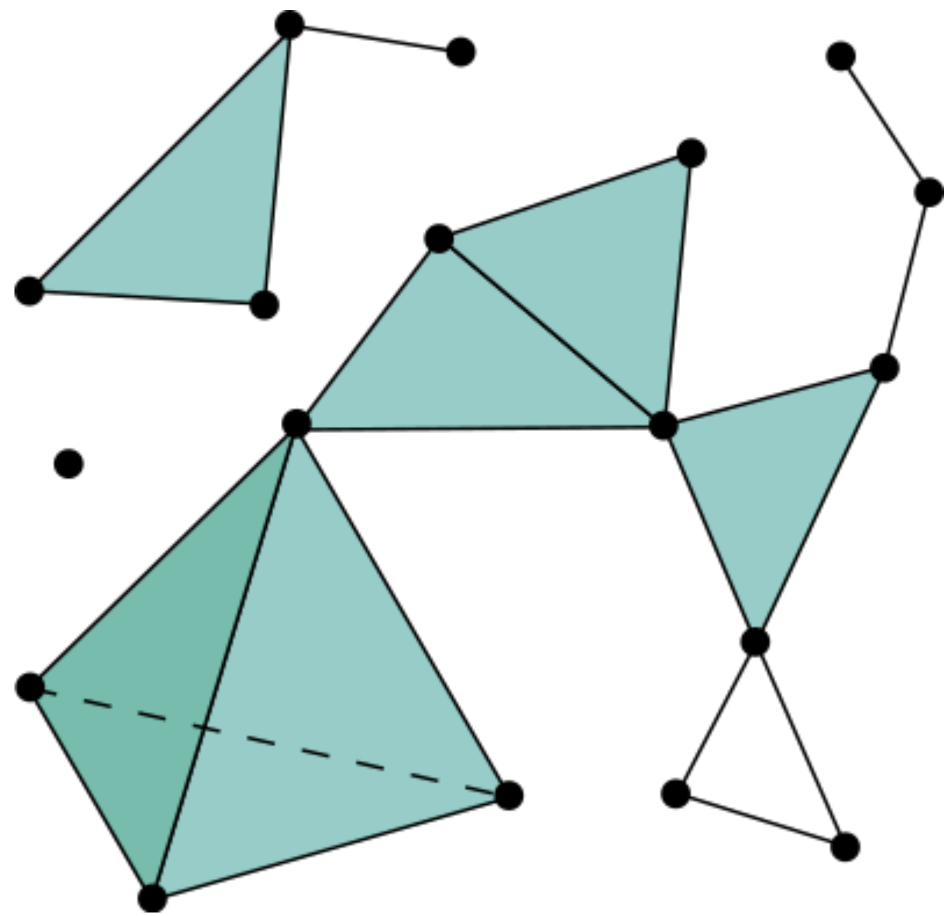
Simplicial complex

Definition:

A ***simplicial complex*** K is a set of simplices that satisfies the two following conditions:

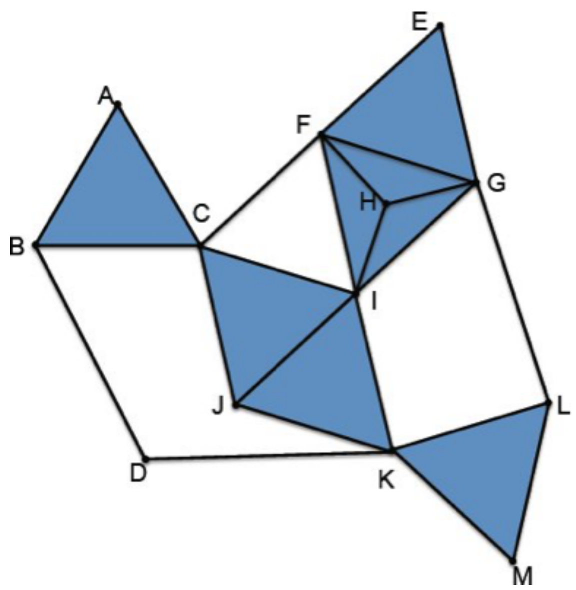
a) Any face of a simplex from K is also in K

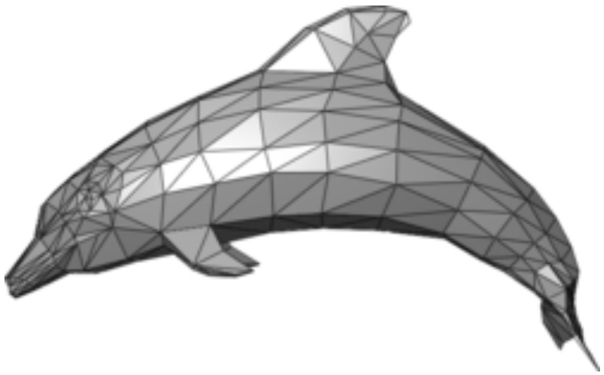
b) The intersection of any two simplices S1 and S2 is either ø or a face of both S1 and S2

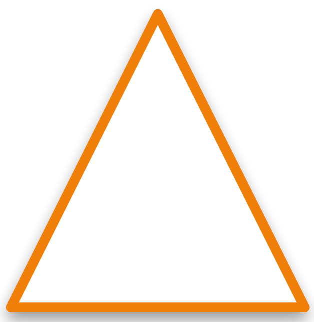


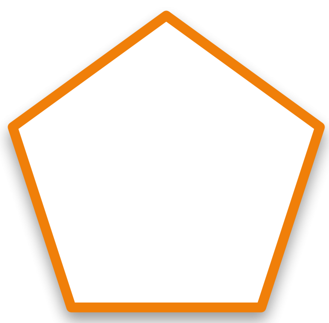
A simplicial 3-complex

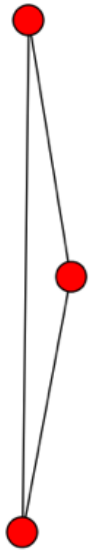
Examples of simplicial complexes



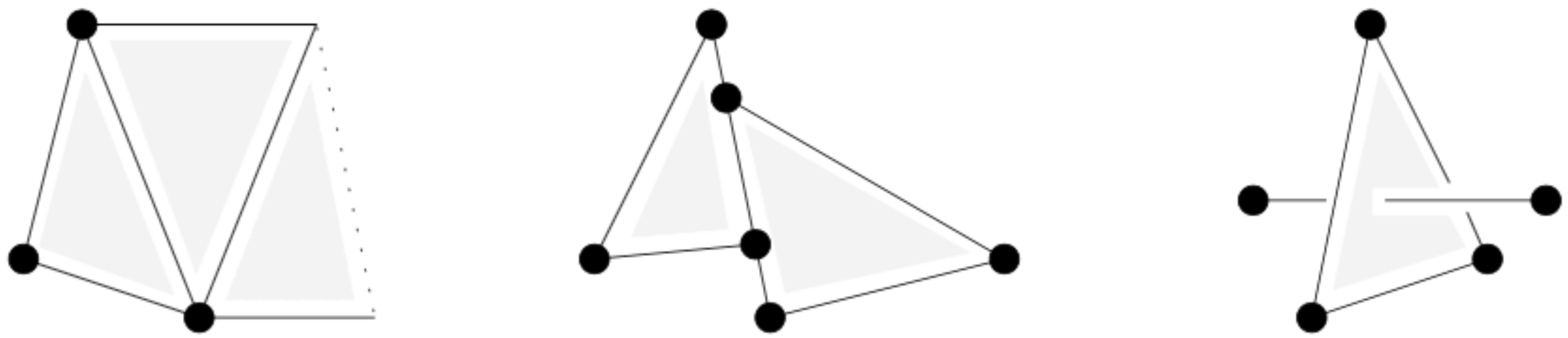




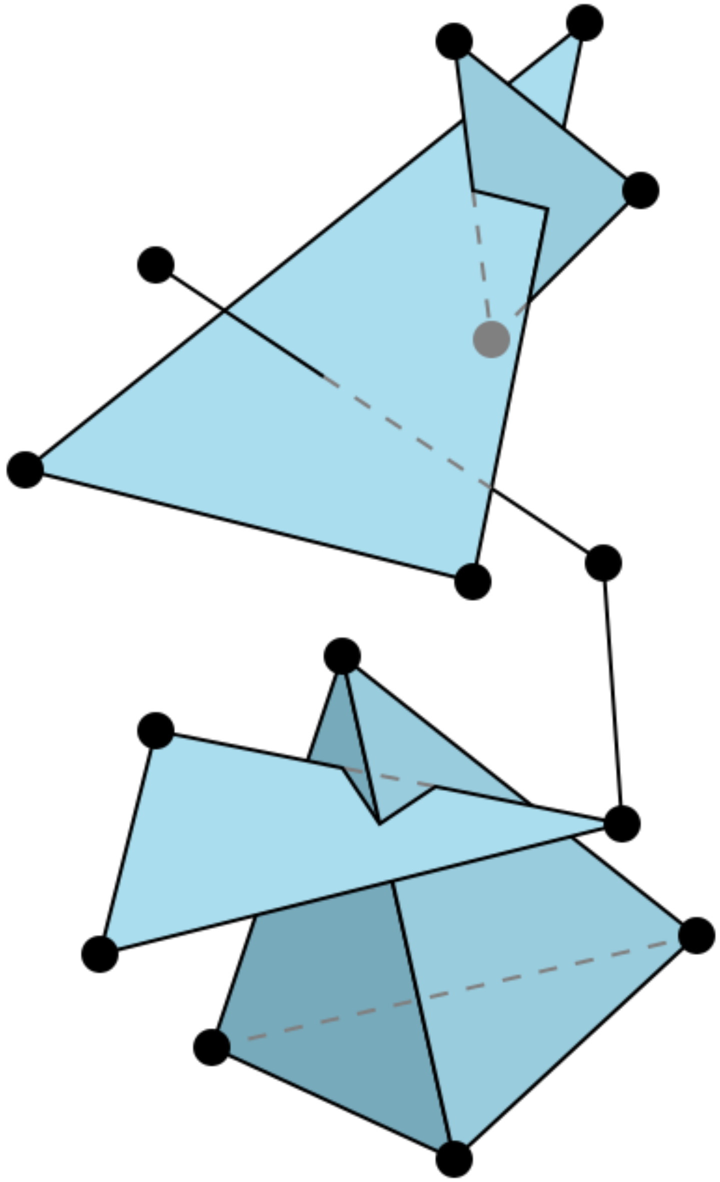




Counter examples of simplicial complexes



Counter examples of simplicial complexes

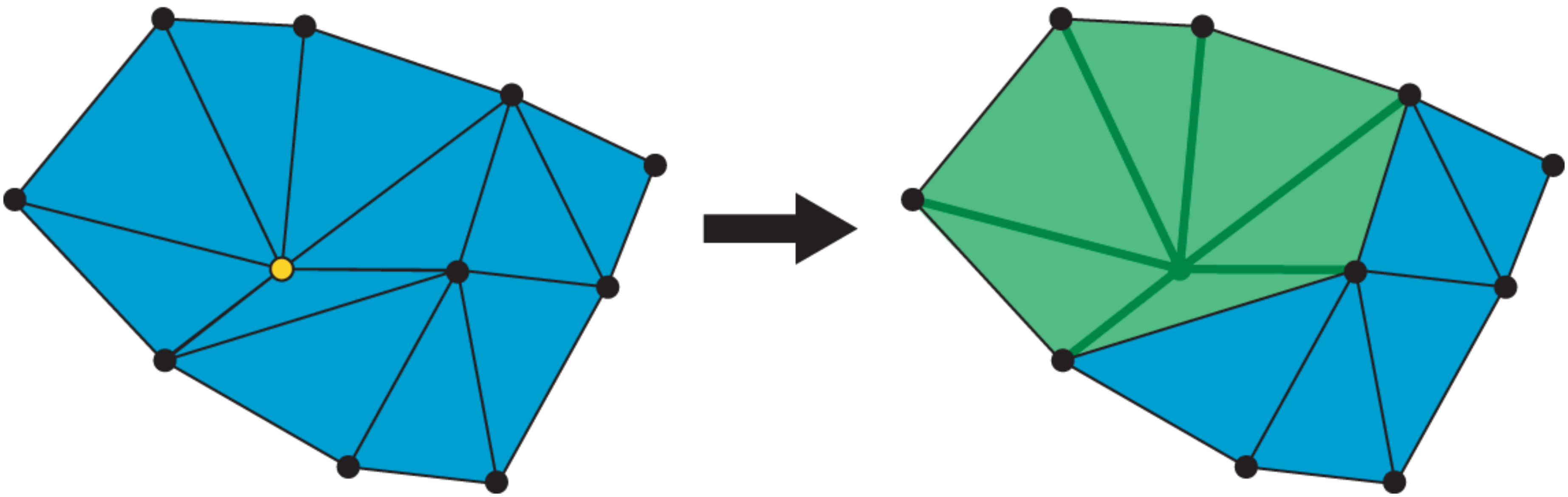


Star in a simplicial complex

Let K be a simplicial complex and S a set of simplices of K.

The ***star*** of S is the union of the stars of all simplices s in S.

The ***star of a simplex s*** is the set of simplices having a face in s.

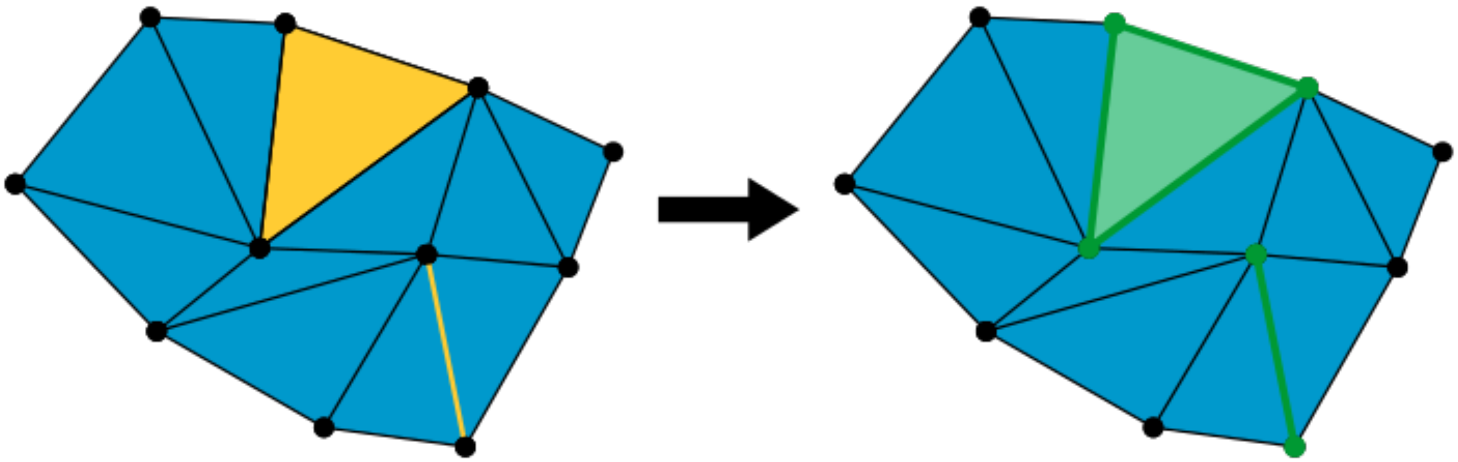


The star of the vertex shown in yellow on the left is the set of the green triangles, edges, and vertices on the right.

Closure in a simplicial complex

Let K be a simplicial complex and S a set of simplices of K.

The ***closure*** of S is is the smallest simplicial subcomplex of K that contains each simplex in S.

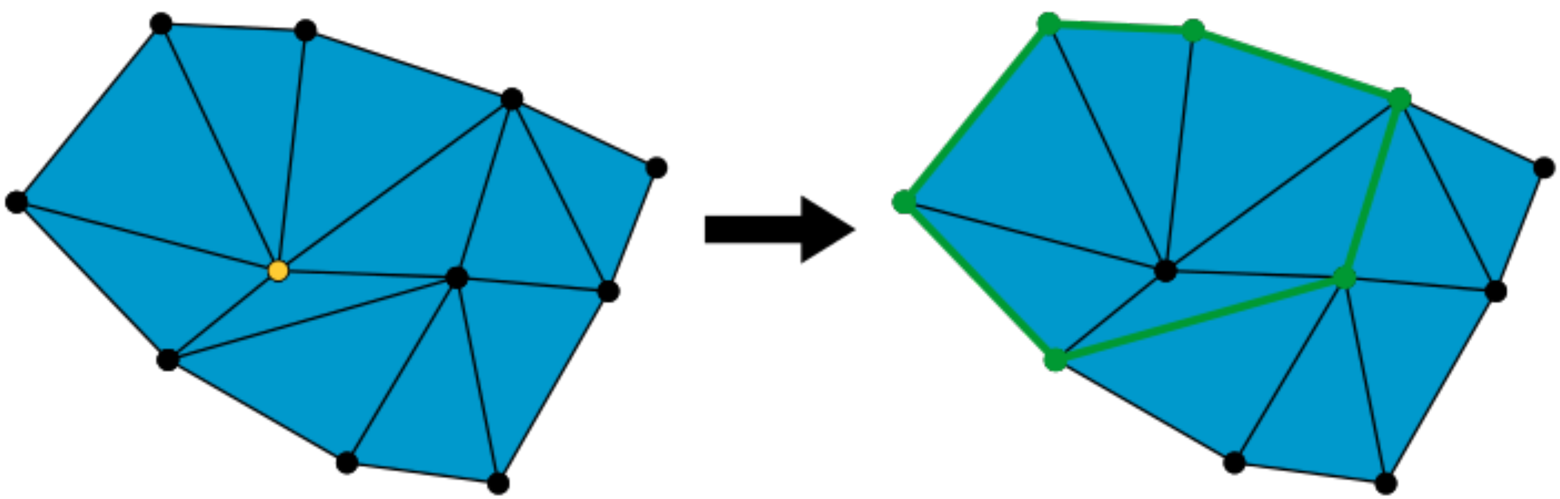


The closure of the simplices shown in yellow on the left is the set of the green triangles, edges, and vertices on the right.

Link in a simplicial complex

Let K be a simplicial complex and S a set of simplices of K.

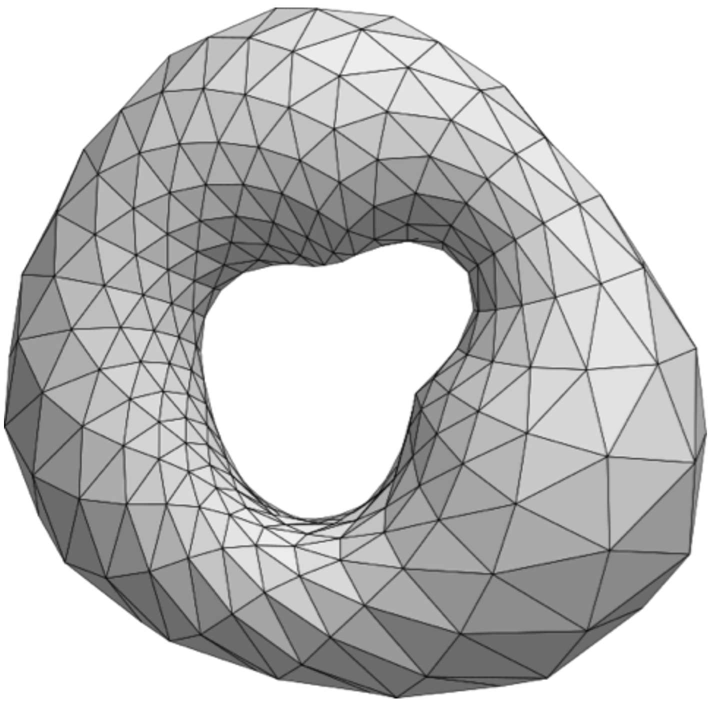
The ***link*** of S is the closed star of S minus the stars of all faces of S.



The link of the vertex shown in yellow on the left is the set of the green edges, and vertices on the right.

Triangulation

Triangulation is the division of a surface or plane polygon into a set of triangles, usually with the restriction that each triangle side is entirely shared by two adjacent triangles. It was proved in 1925 that every surface has a triangulation, but it might require an infinite number of triangles and the proof is difficult.



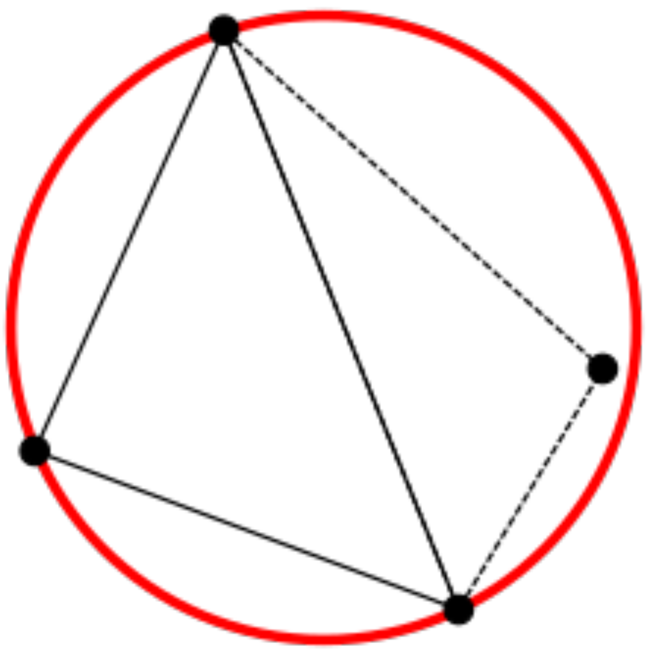
A triangulation of the torus

Delaunay Triangulation

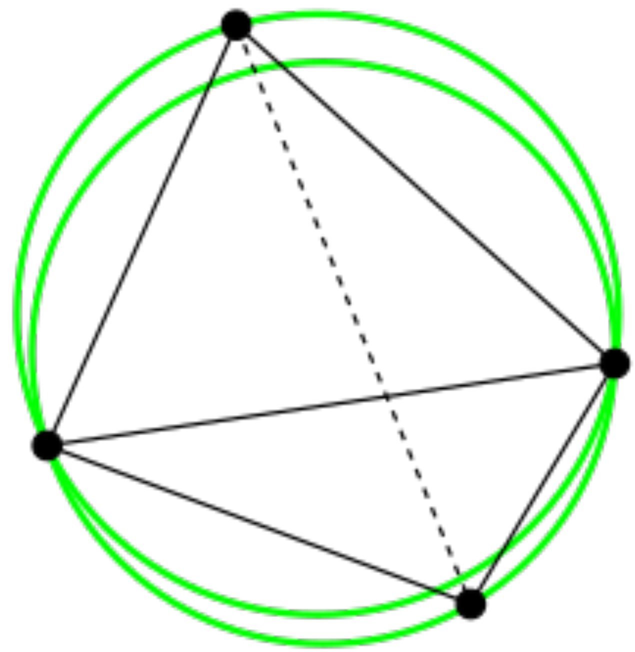
A **Delaunay triangulation** for a set **P** of points in a plane is a triangulation DT(**P**) such that no point in **P** is inside the circumcircle of any triangle in DT(**P**).

Delaunay triangulations maximize the minimum angle of all the angles of the triangles in the triangulation

Delaunay Triangulation: edge flipping



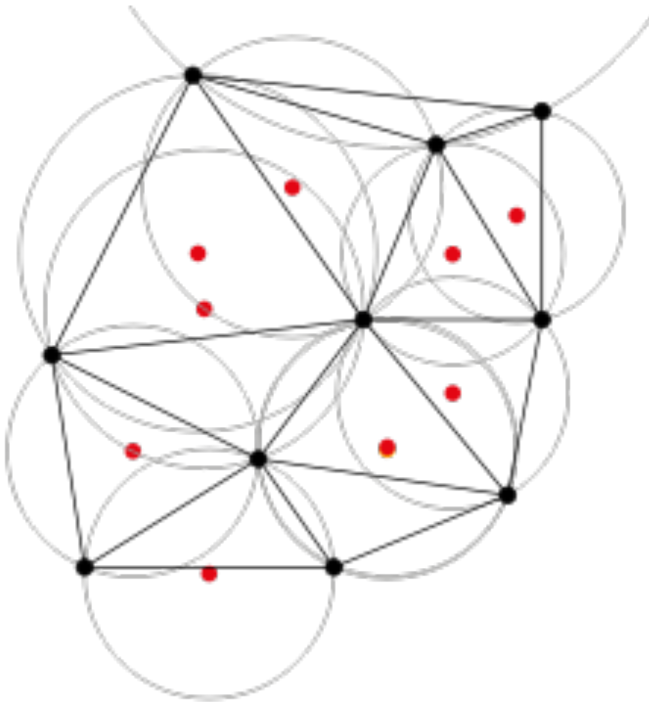
This pair of triangles does not meet the Delaunay condition (the circumcircle contains more than three points).



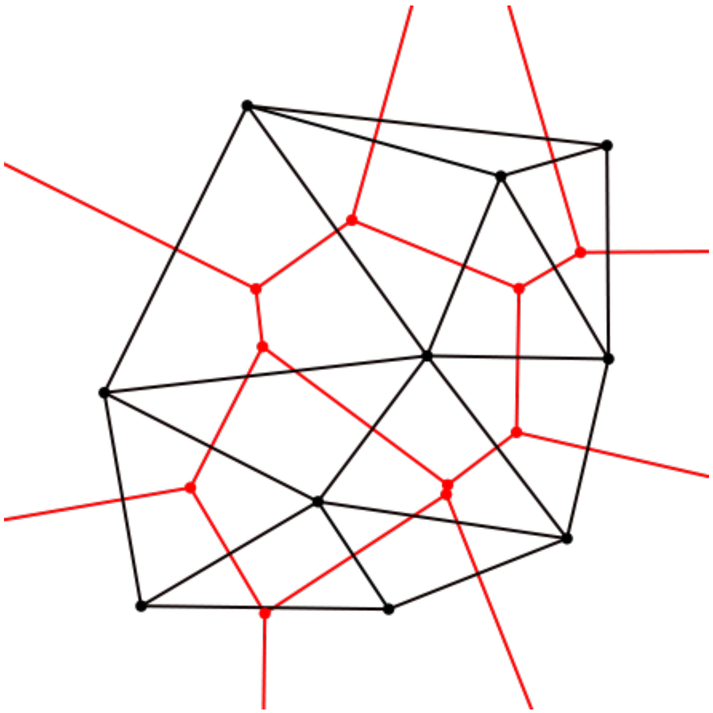
Flipping the common edge produces a valid Delaunay triangulation for the four points

Delaunay Triangulation and Voronoi Diagram

The Delaunay triangulation of a discrete point set **P** in general position corresponds to the dual graph of the Voronoi diagram for **P**

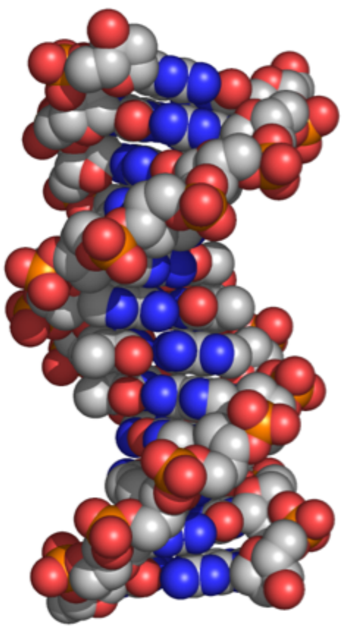


The Delaunay triangulation with all the circumcircles and their centers (in red)



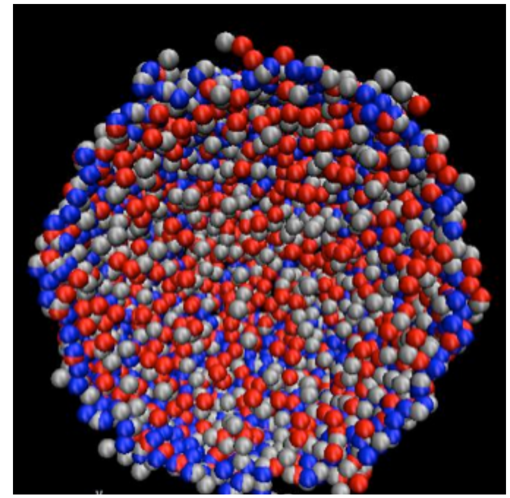
Connecting the centers of the circumcircles produces the Voronoi diagram (in red).

Sphere Representations in Biology

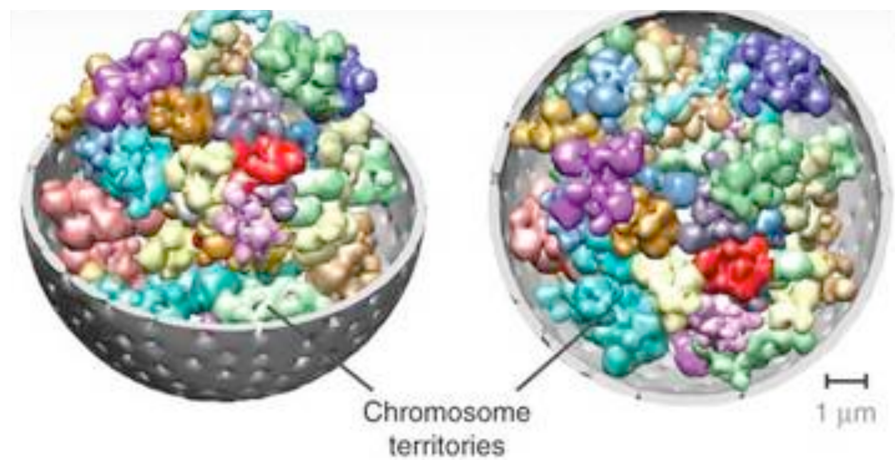


DNA

Nucleosome

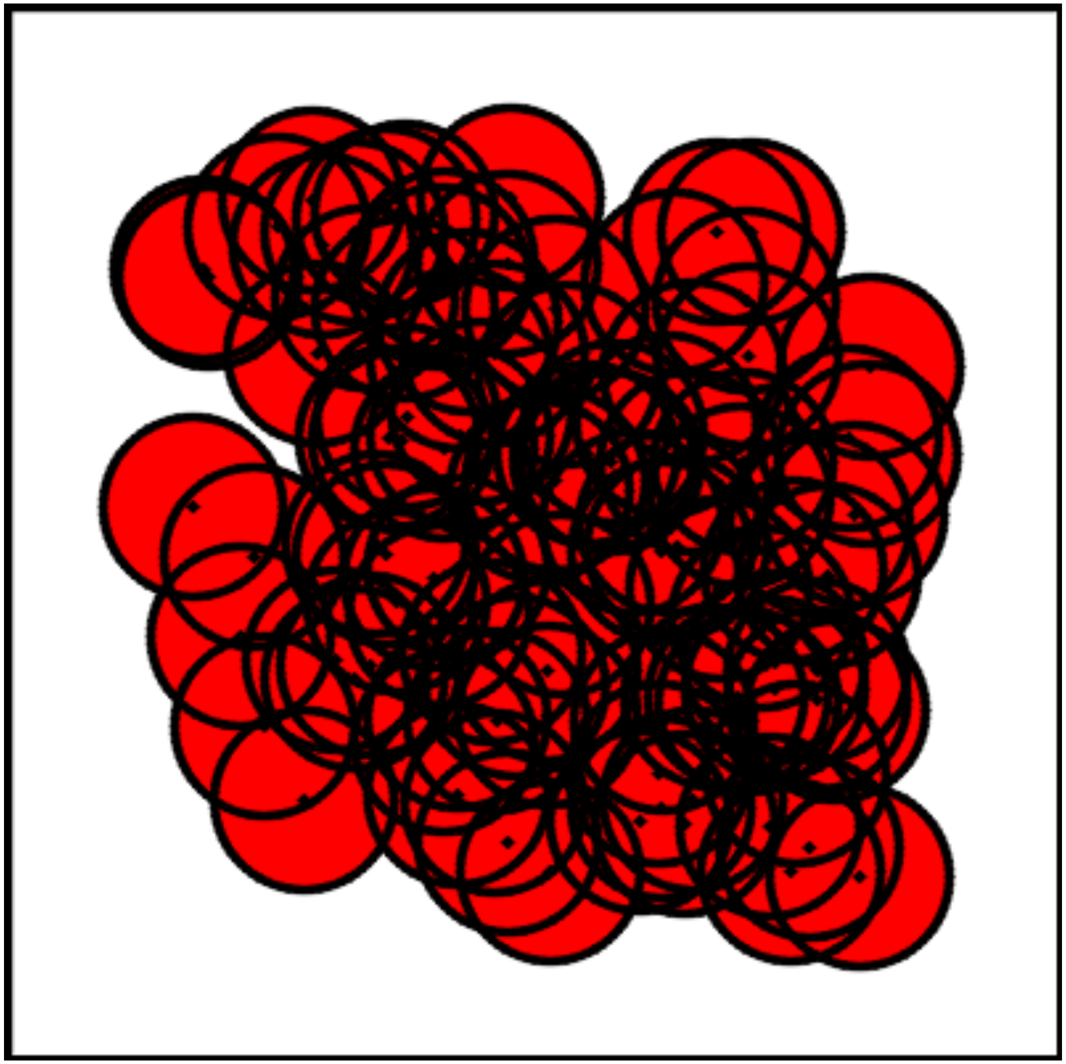


Viral DNA

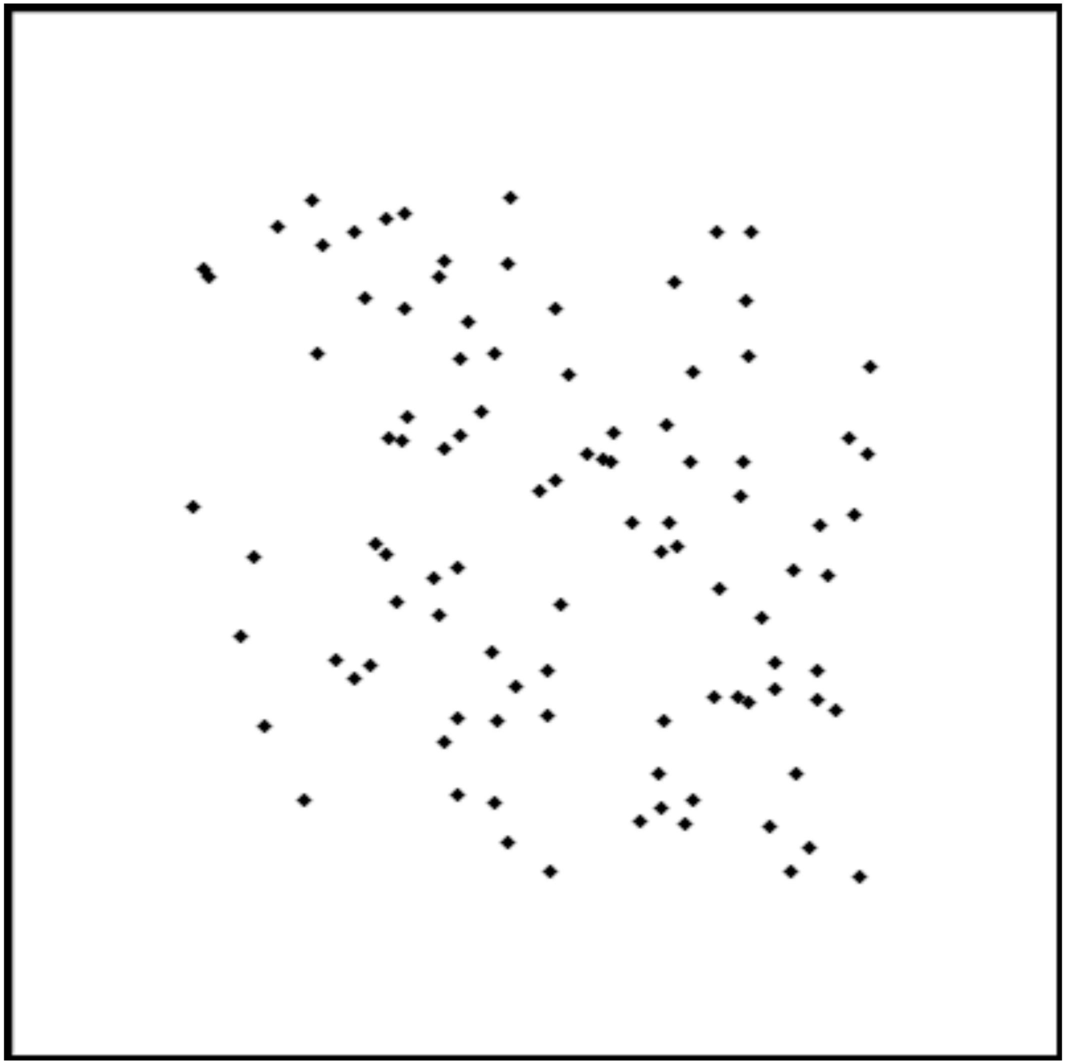


Chromosome arrangements

Measuring a Union of Balls



Measuring a Union of Balls



Measuring a Union of Balls

Algorithm for computing Delaunay triangulation:

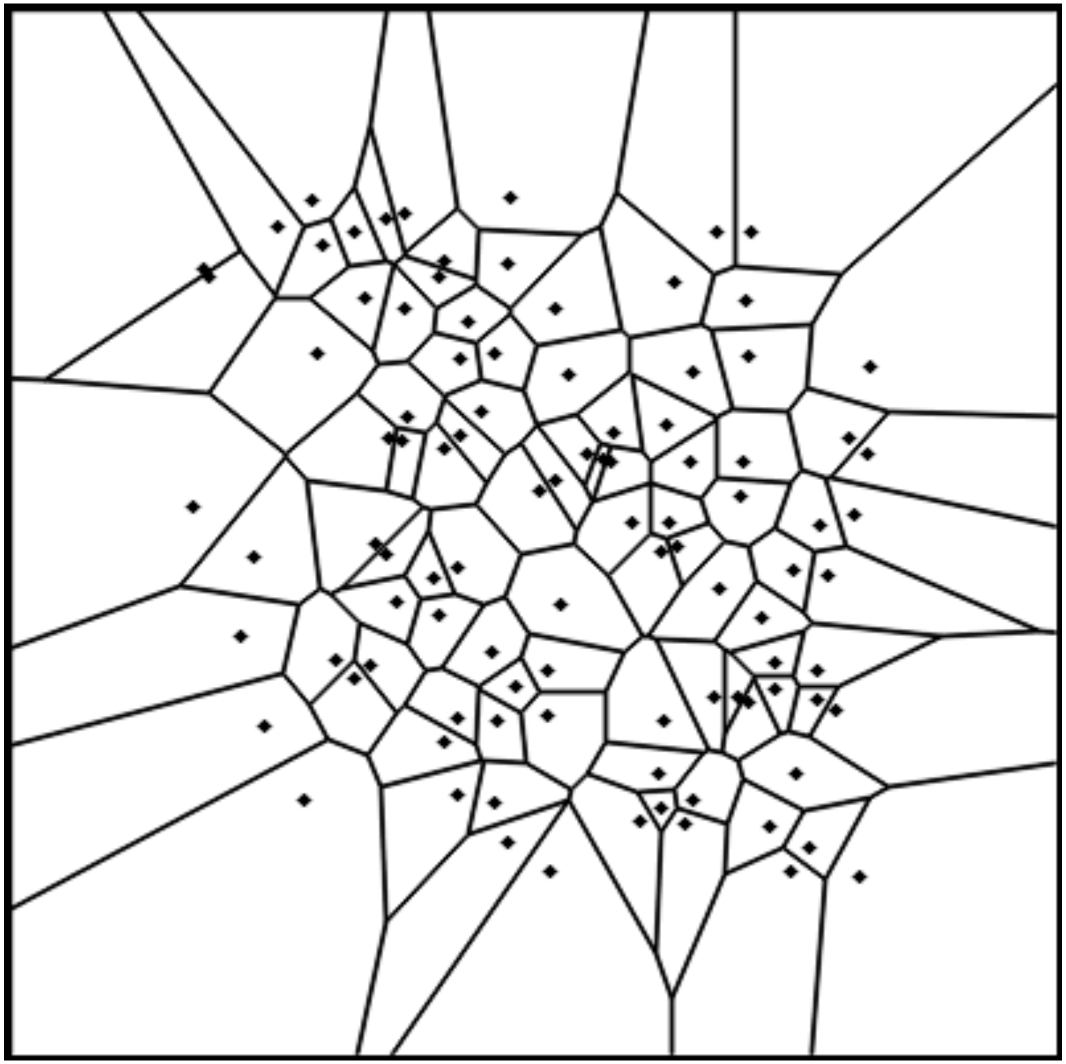
Input: N: number of points
Ci: position of point I

1) Randomize points

2) For i = 1:N
   - **Location**: find triangle t that contains Ci
   - **Addition**: Divide t into 3 triangles
   - **Correct**: flip non local triangles

Output: list of triangles

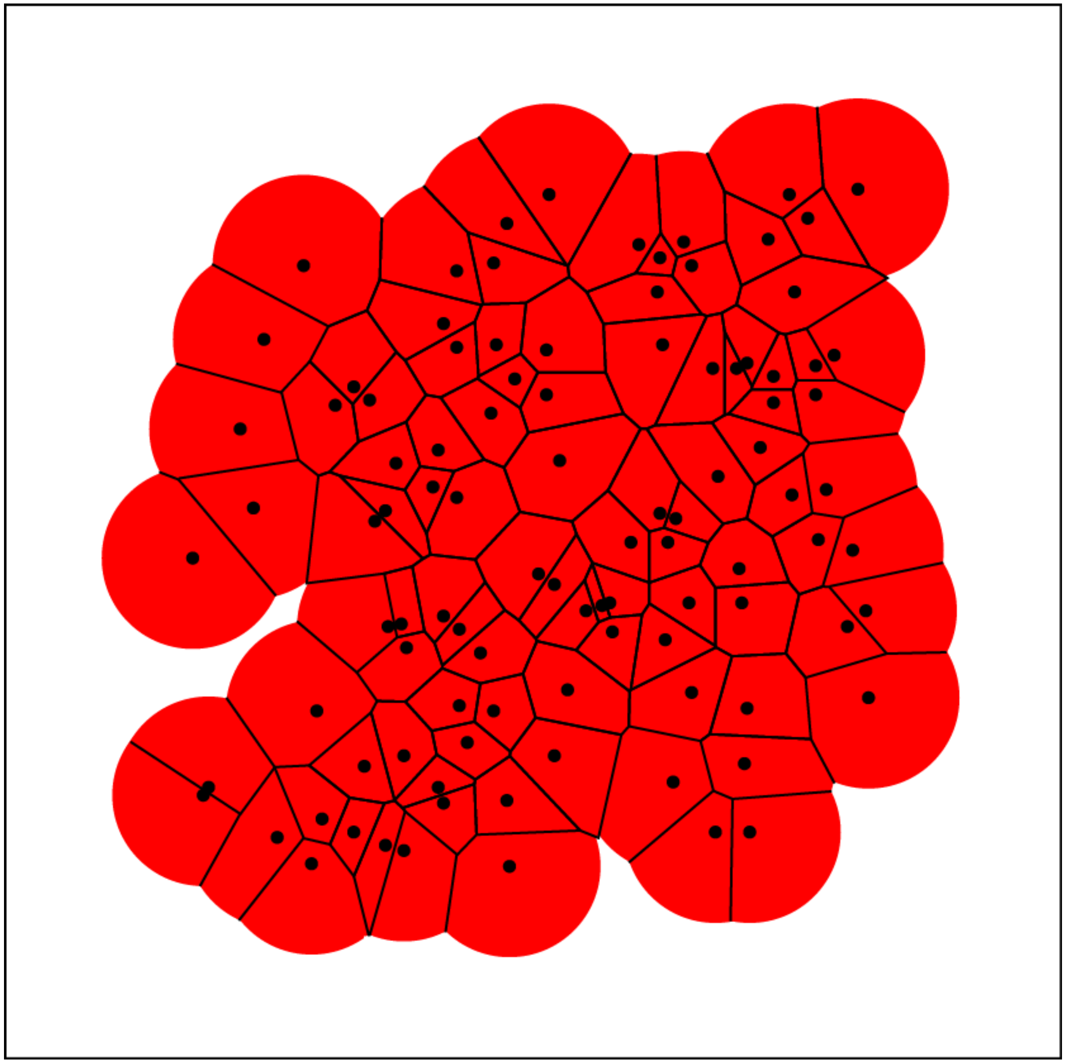
Measuring a Union of Balls



Compute Voronoi diagram from

Delaunay complex: dual

Measuring a Union of Balls

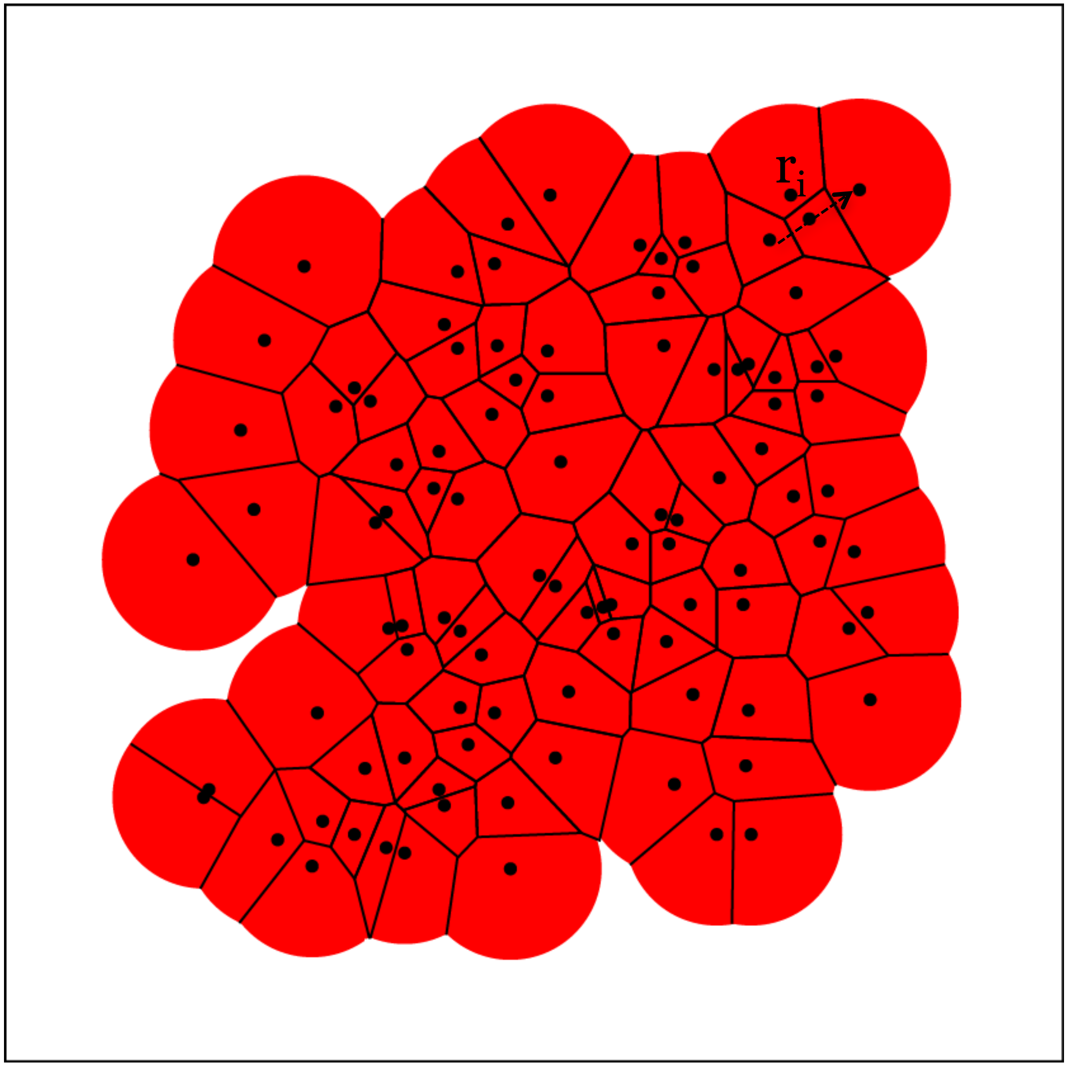


Restrict Voronoi diagram to

the Union of Balls:

Power diagram

Measuring a Union of Balls



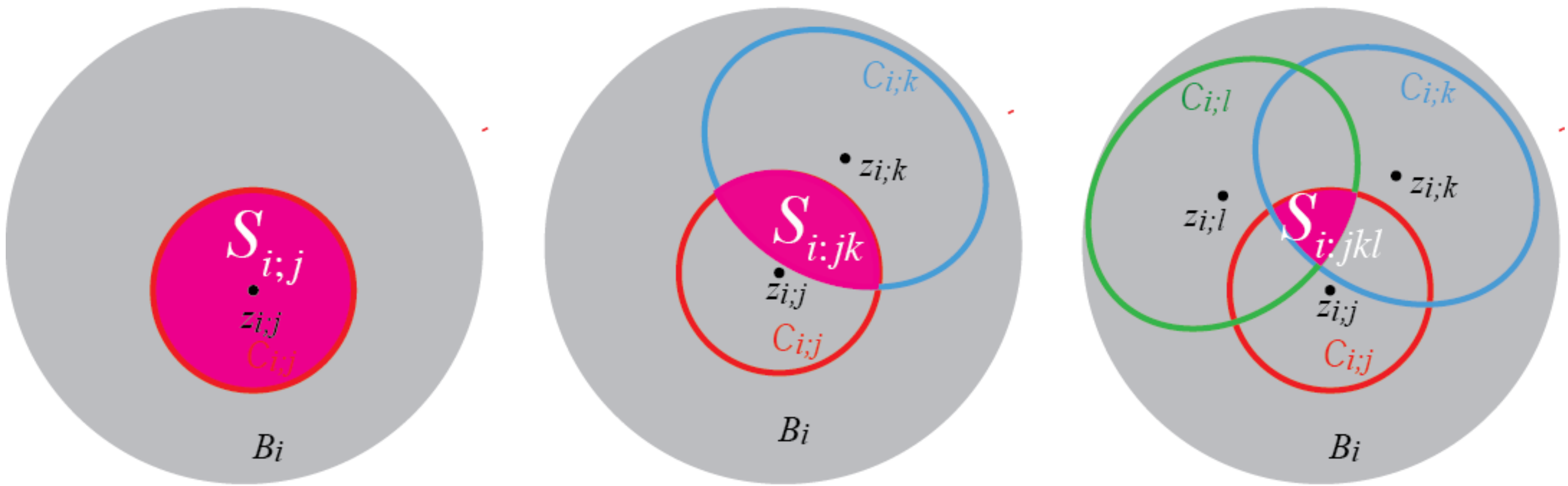
Atom i:
Fraction in Voronoi cell:
σ_i and β_i

$$A_i = 4\pi \sum_{i=1}^{N} r_i^2 \sigma_i$$

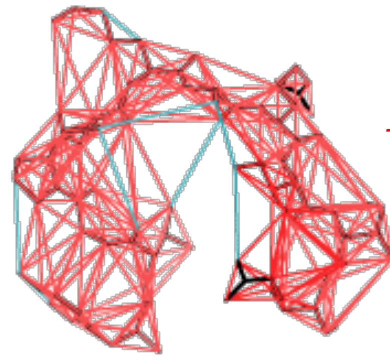
$$V_i = \frac{4\pi}{3} \sum_{i=1}^{N} r_i^3 \beta_i$$

Measuring a Union of Balls

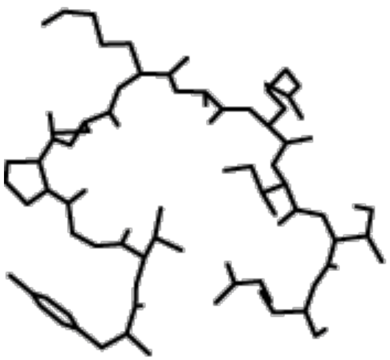
$$A_i = S_i - S_{i;j} - S_{i:k} - S_{i:l} + S_{i:jk} + S_{i:jl} + S_{i:kl} - S_{i:jkl}$$



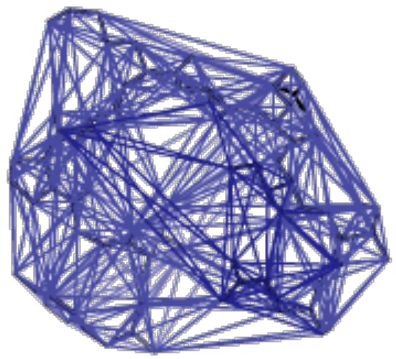
Measuring a Union of Balls



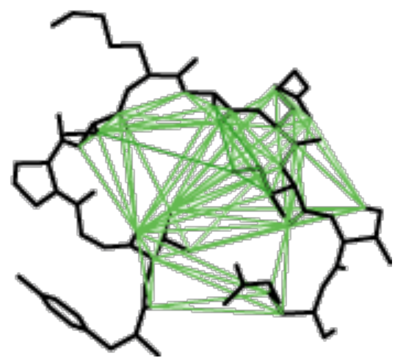
K complex



Protein

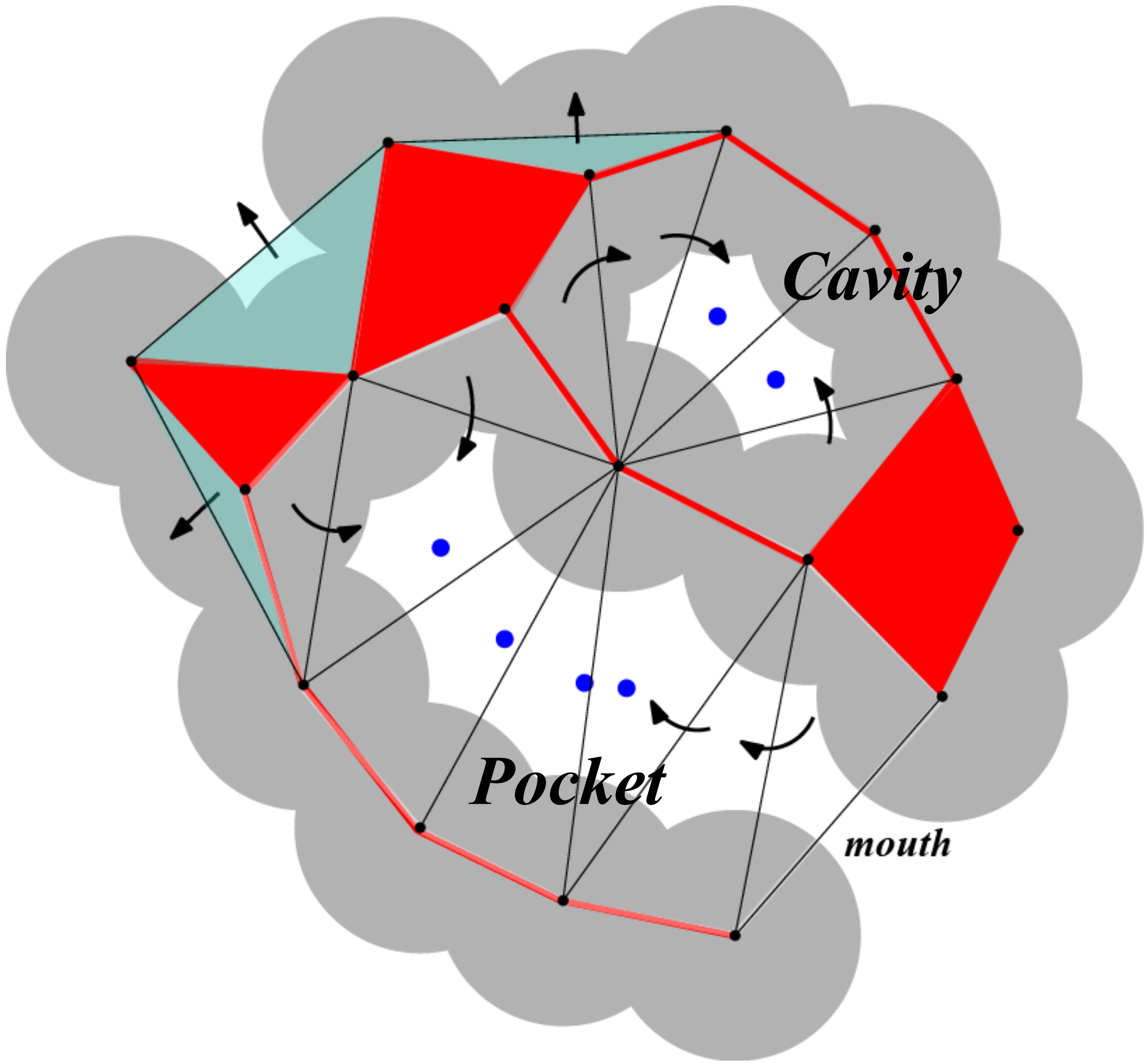


Delaunay Complex

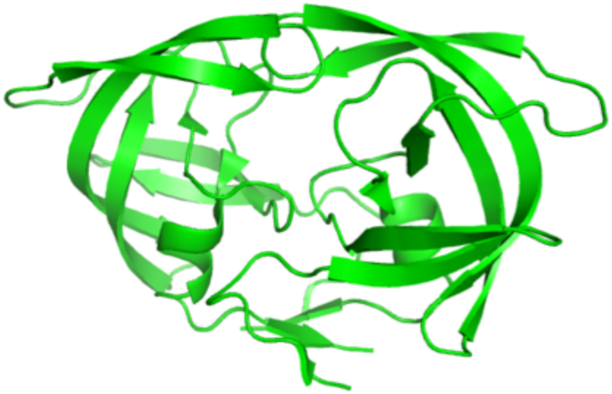


Pocket

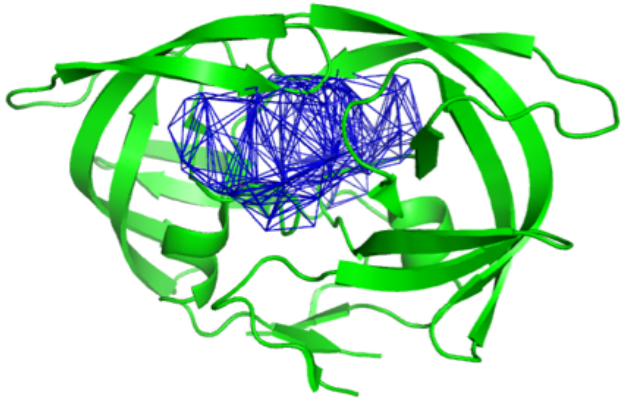
Measuring a Union of Balls



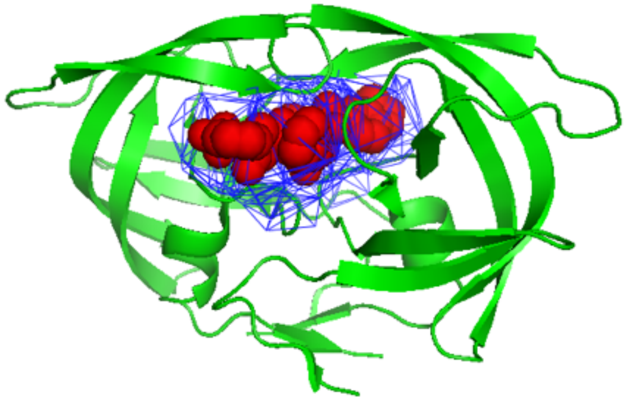
Applications to drug design



HIV protease (3MXE)



Main cavity



Actual position of K54 (inhibitor)

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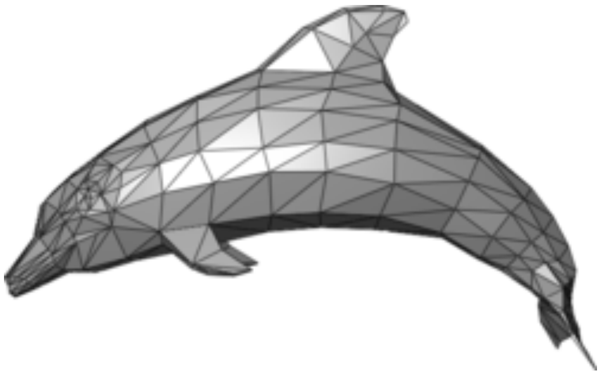
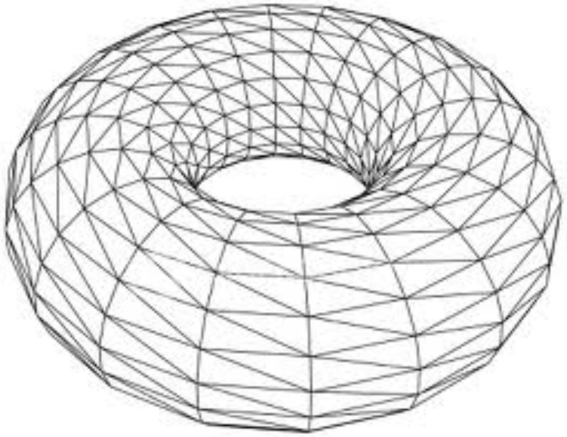
Polygonal meshes

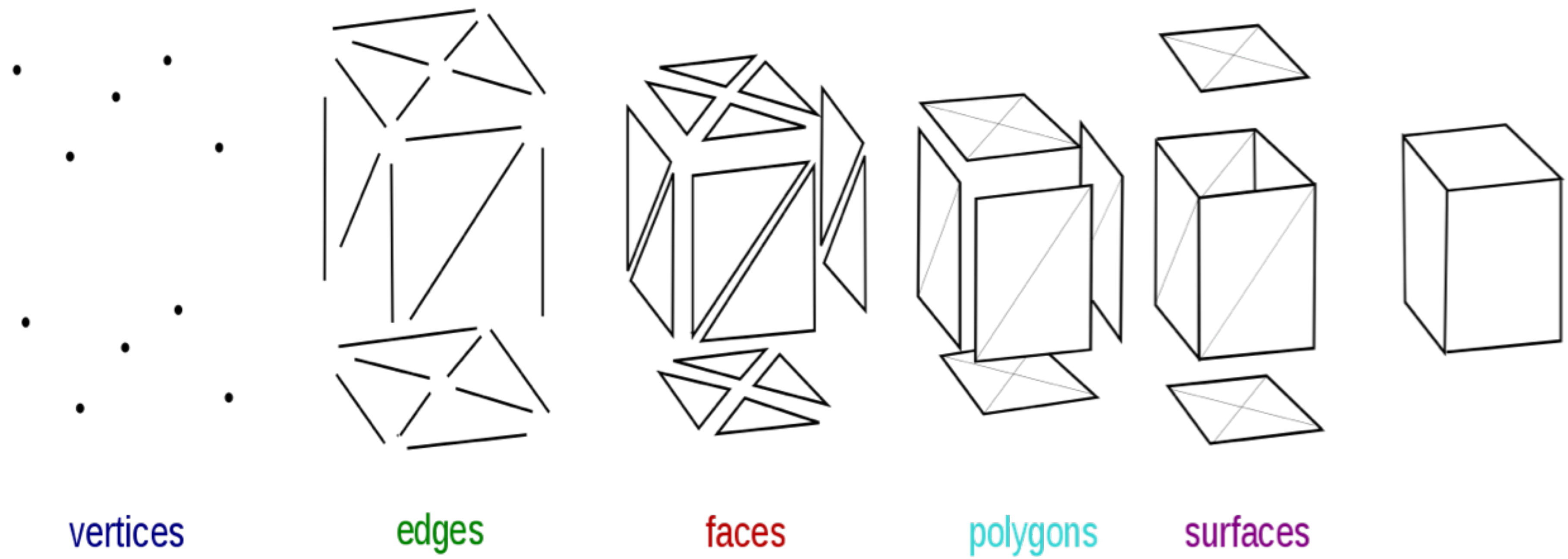
A polygon mesh is a collection of vertices, edges and faces that defines the shape of a polyhedral object



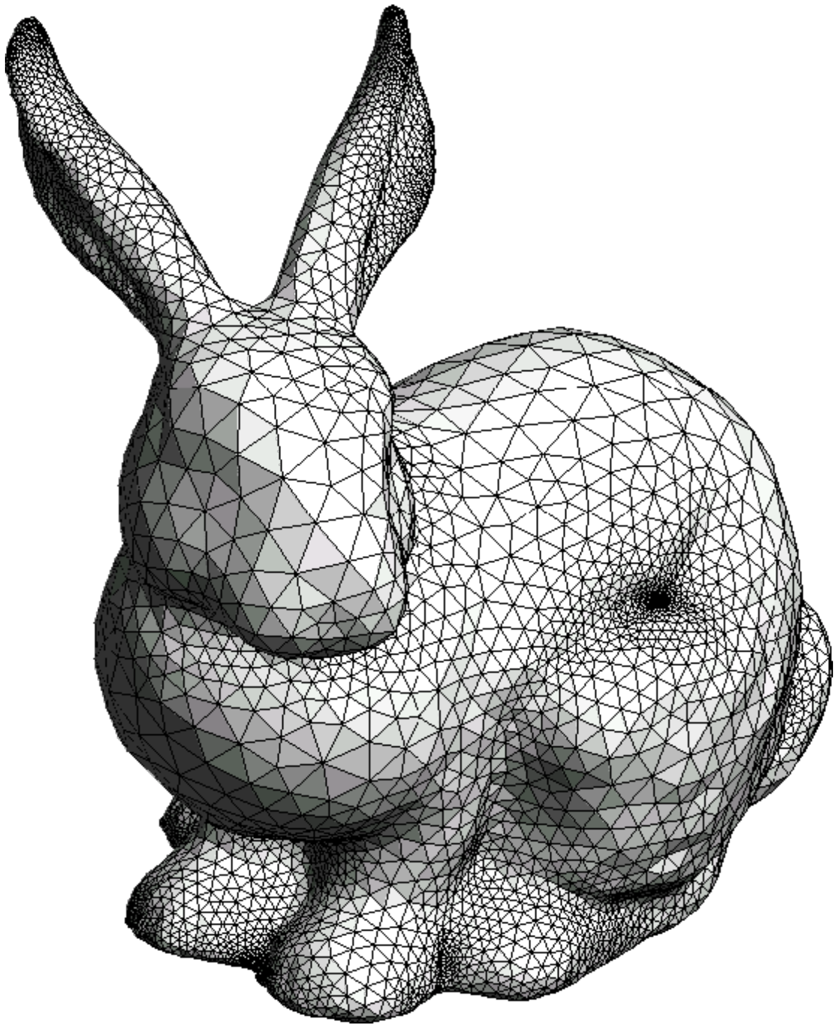


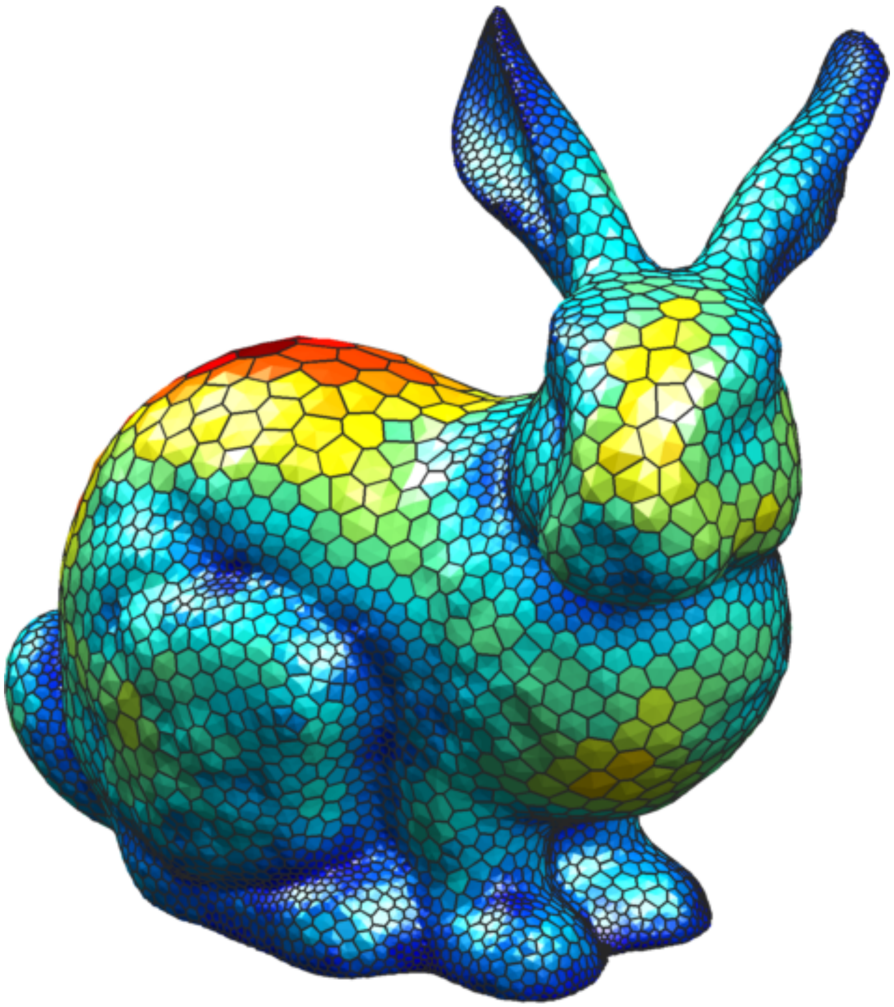
The faces usually consist of triangles (triangle mesh), quadrilaterals, or other simple convex polygons, since this simplifies rendering.

Polygonal meshes



Polygonal meshes

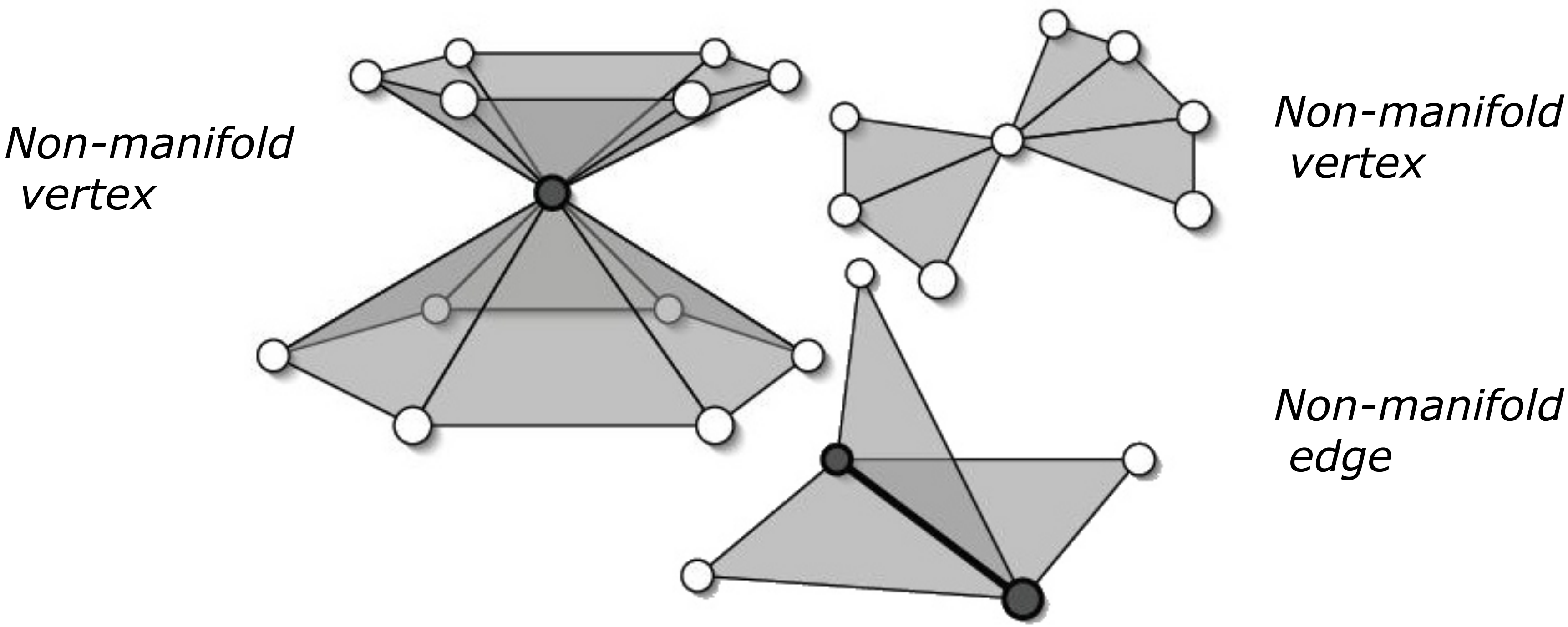




Some definitions about meshes

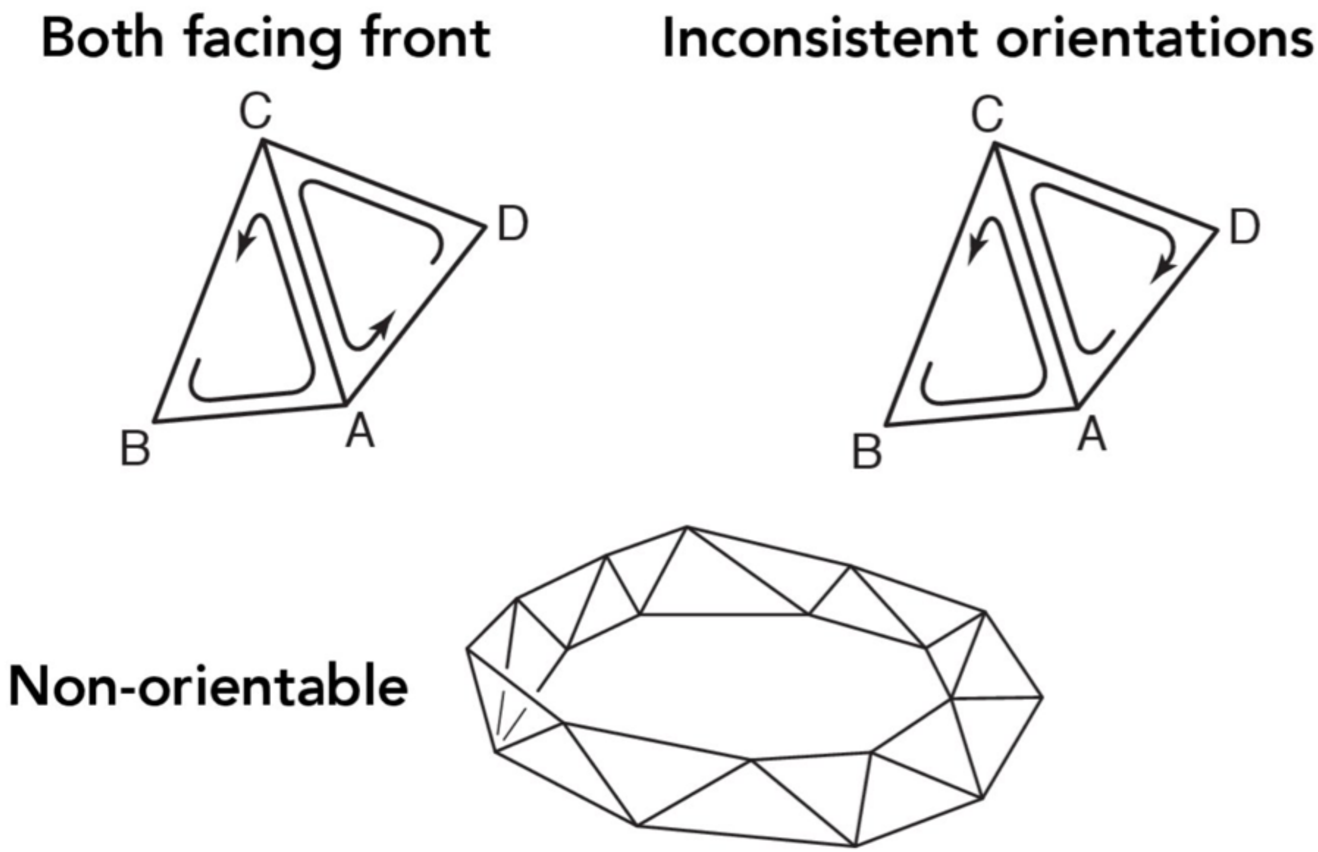
degenerate: contains duplicate triangles
(i.e. the same three vertices describe two triangles) ,
or triangles with two or three overlapping vertices.

manifold: no vertex is adjacent to more than two boundary edges,
and no edge is shared by more than two triangles.



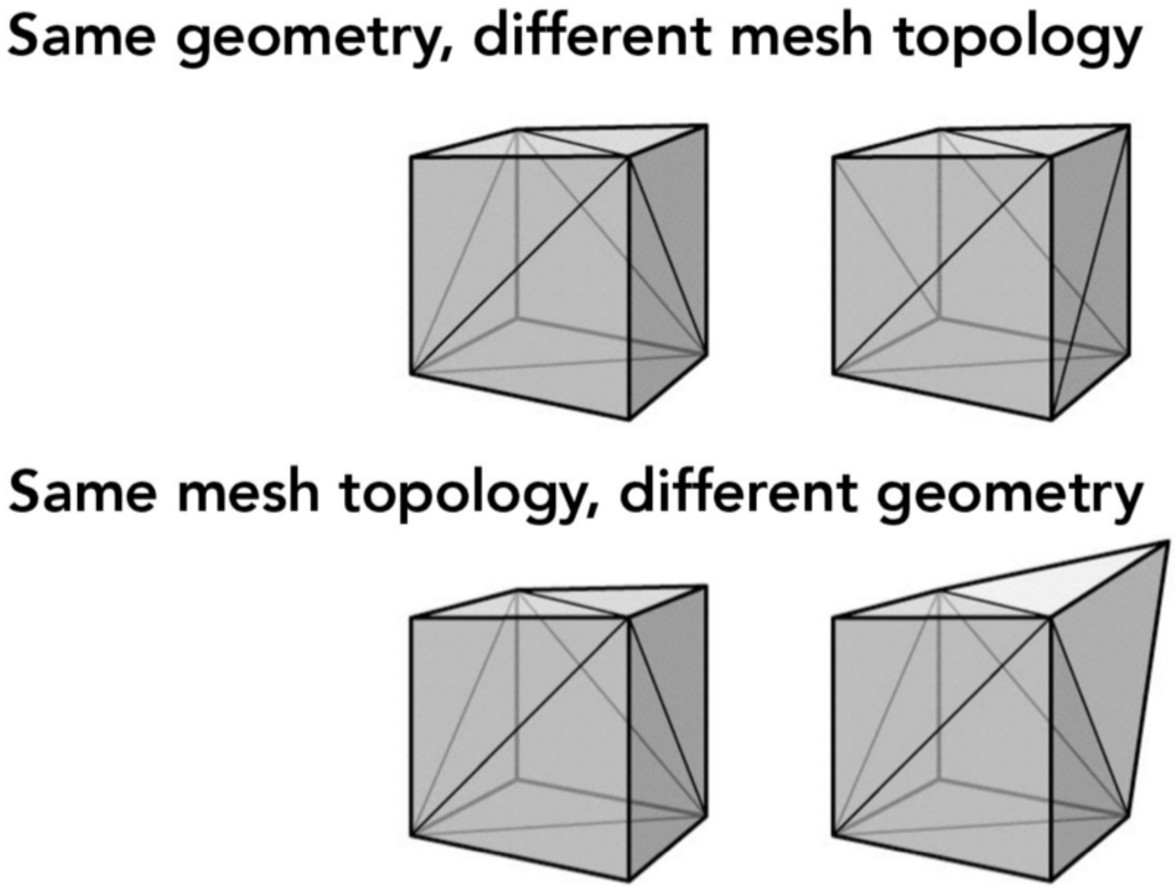
Some definitions about meshes

orientable: a mesh is orientable if all normals of the triangles can be made compatible



Meshes: geometry and topology

The **topology** of a mesh is given by the combinatorics of its edges and triangles
The **geometry** of a mesh is given by the position (coordinates) of its vertices and/or lengths of its edges.



Euler formula for triangular meshes

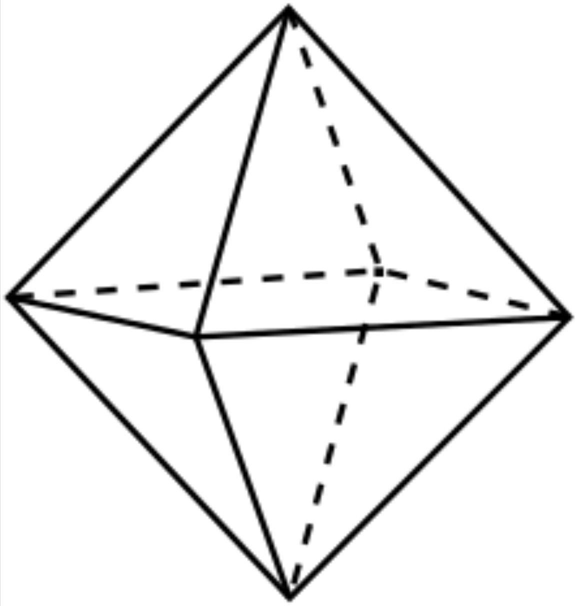
Let M be a mesh that contains V vertices, E edges, T triangles, B edges at its boundaries (if any), and C components. Let us assume that this mesh represents a surface of genus g. Then the following formula is true:

$$V - E + T = 2(C - g) - B$$

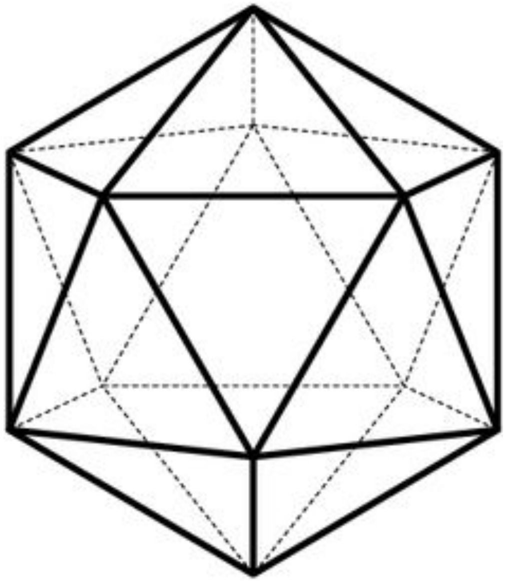
Most common meshes:
C = 1 (a single component), B=0 (no boundaries), g = 0 (genus 0, i.e. topologically equivalent to the sphere); then:

$$V - E + T = 2$$

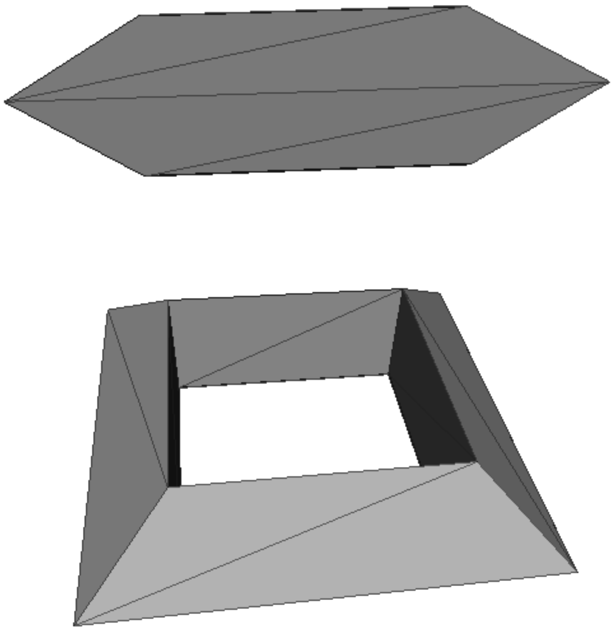
Examples



V =
E =
T =
V-E+T =

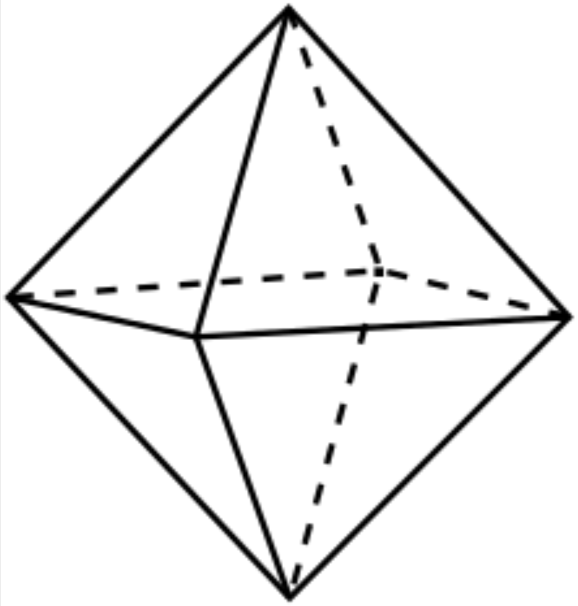


V =
E =
T =
V-E+T =

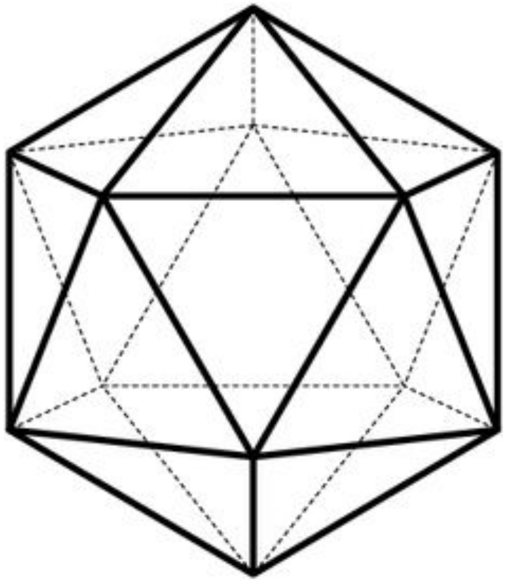


V =
E =
T =
V-E+T =

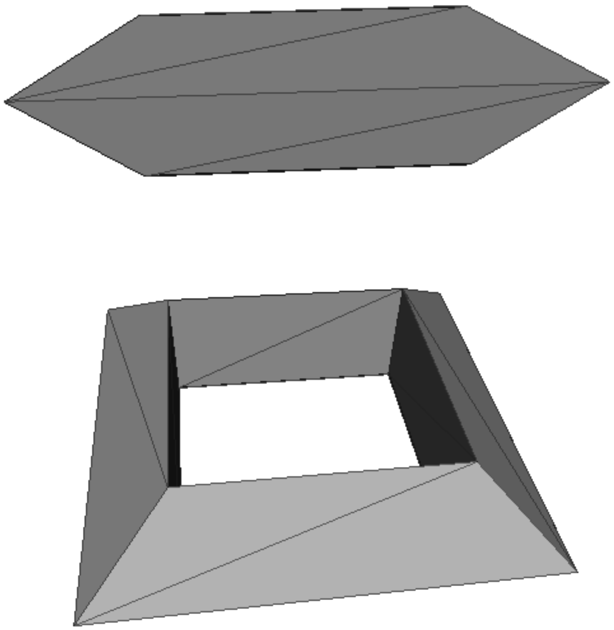
Examples



V = 6
E = 12
T = 8
V-E+T =2



V = 12
E = 30
T = 20
V-E+T = 2



V = 12
E = 36
T = 24
V-E+T = 0 !

Discrete representations of shapes

1) **Continuous surfaces**
   1) Manifolds
   2) Metric on manifolds
   3) Topology
   4) Orientation

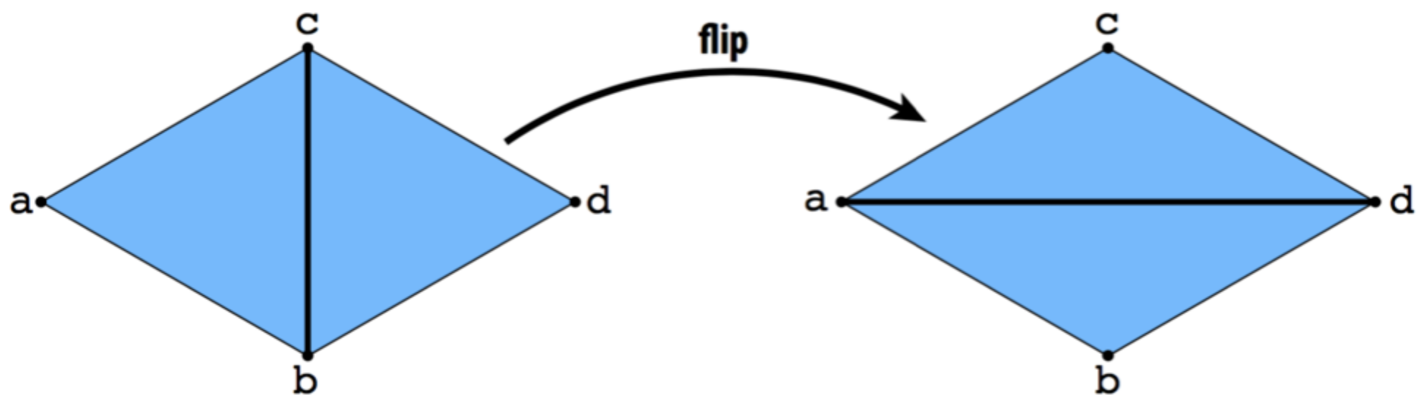
2) **Sets of points and triangulations**
   1) Simplicial complexes
   2) Triangulations
   3) Delaunay and applications

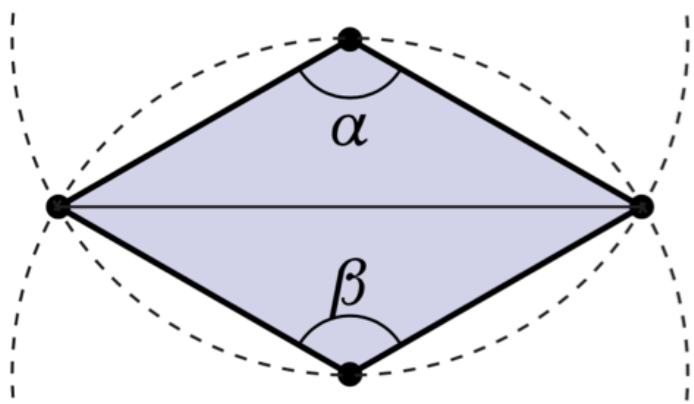
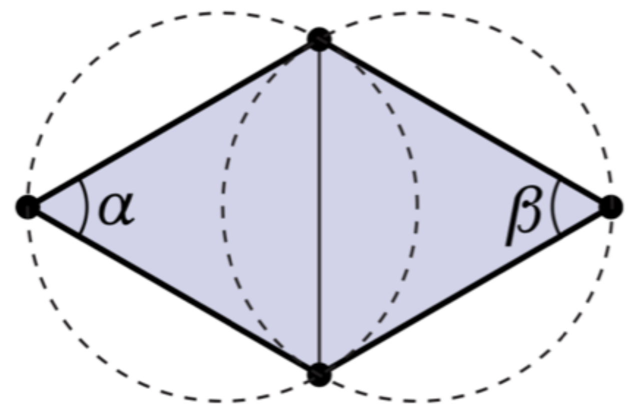
3) **Discrete Surfaces**
   1) Meshes
   2) Manifold/ orientation
   3) Geometry / topology

4) **Manipulating discrete surfaces**
   1) Basic mesh operations
   2) Remeshing

Basic mesh operations

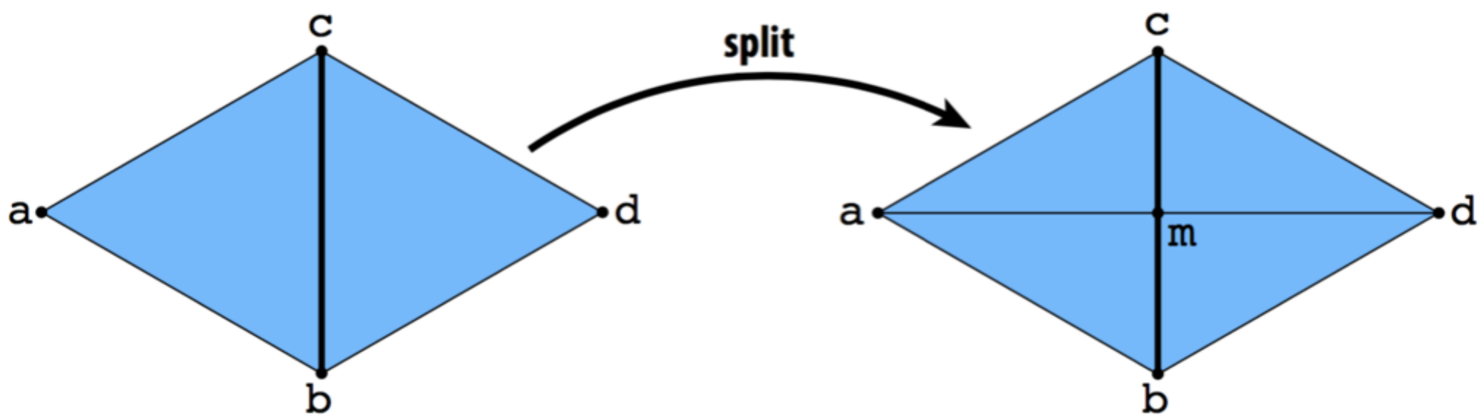
1. **Edge flip:** triangles (a,b,c) and (b,c,d) become (a,c d) and (a,b,d)



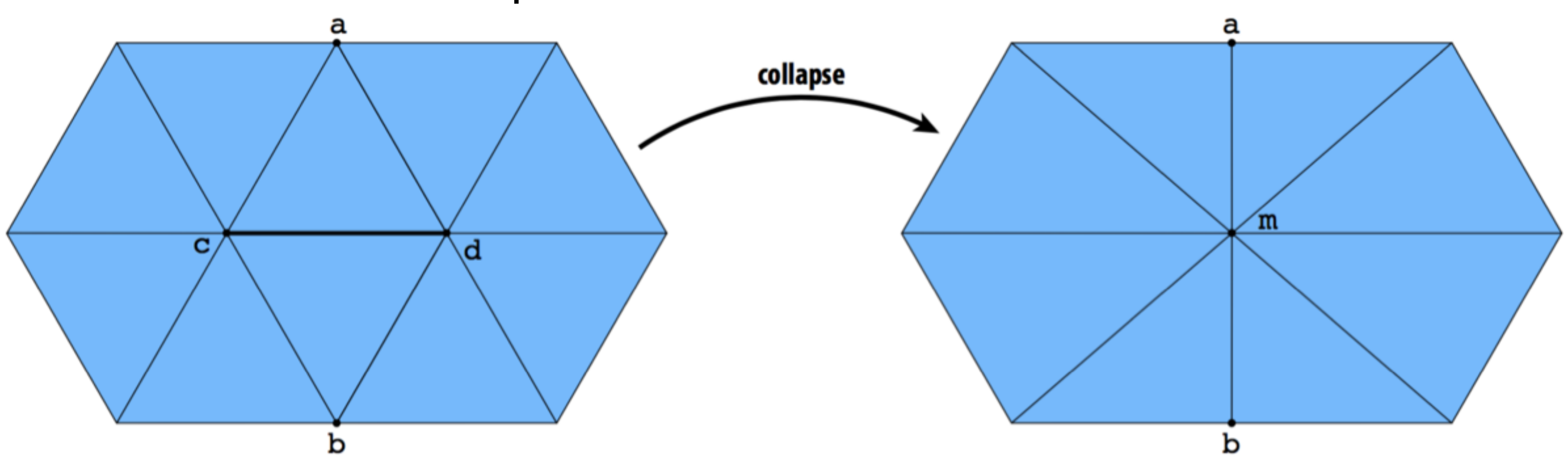

α
β

α
β

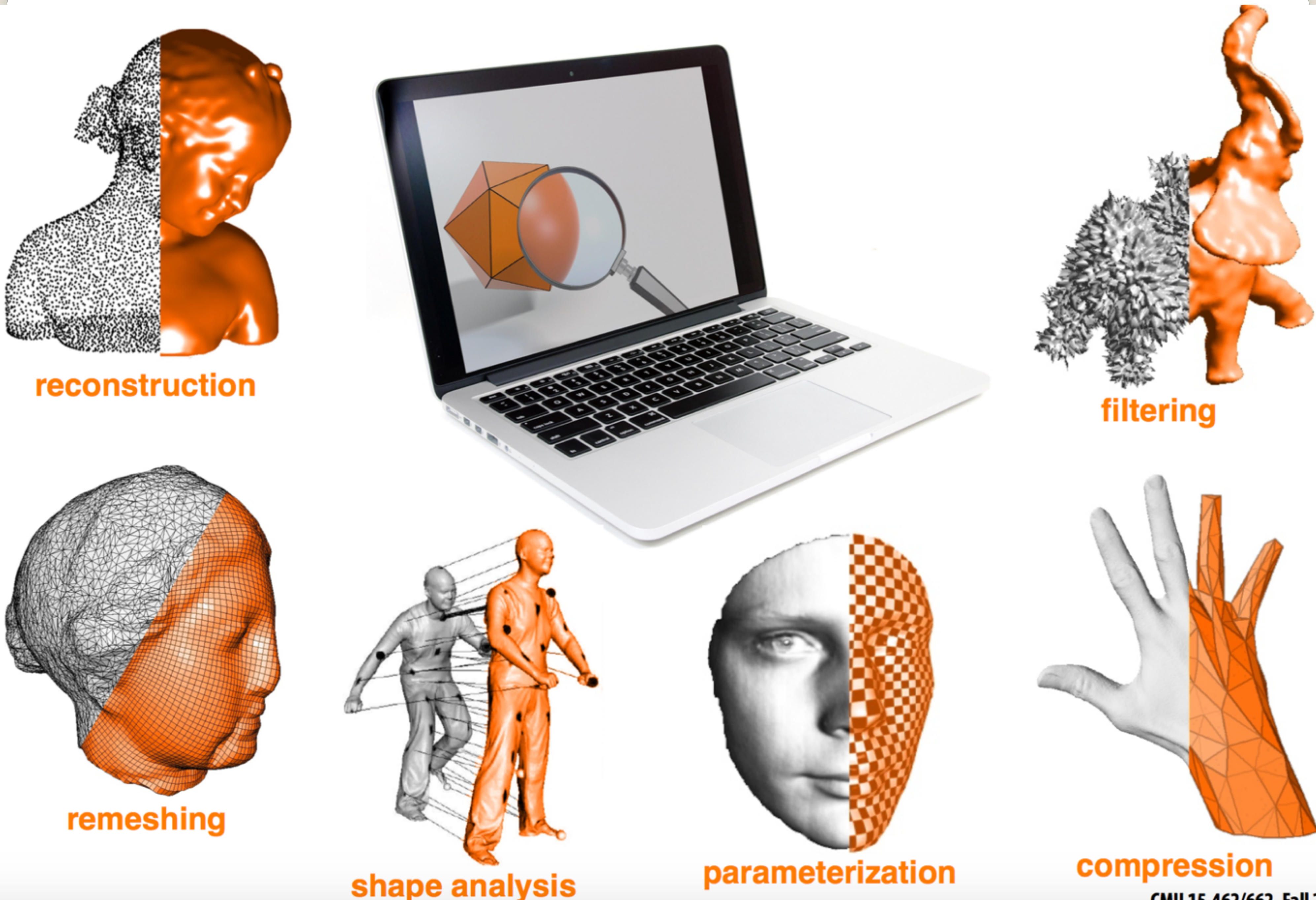
Basic mesh operations

2. Edge split: add midpoint of edge (b,c) and form 4 triangles

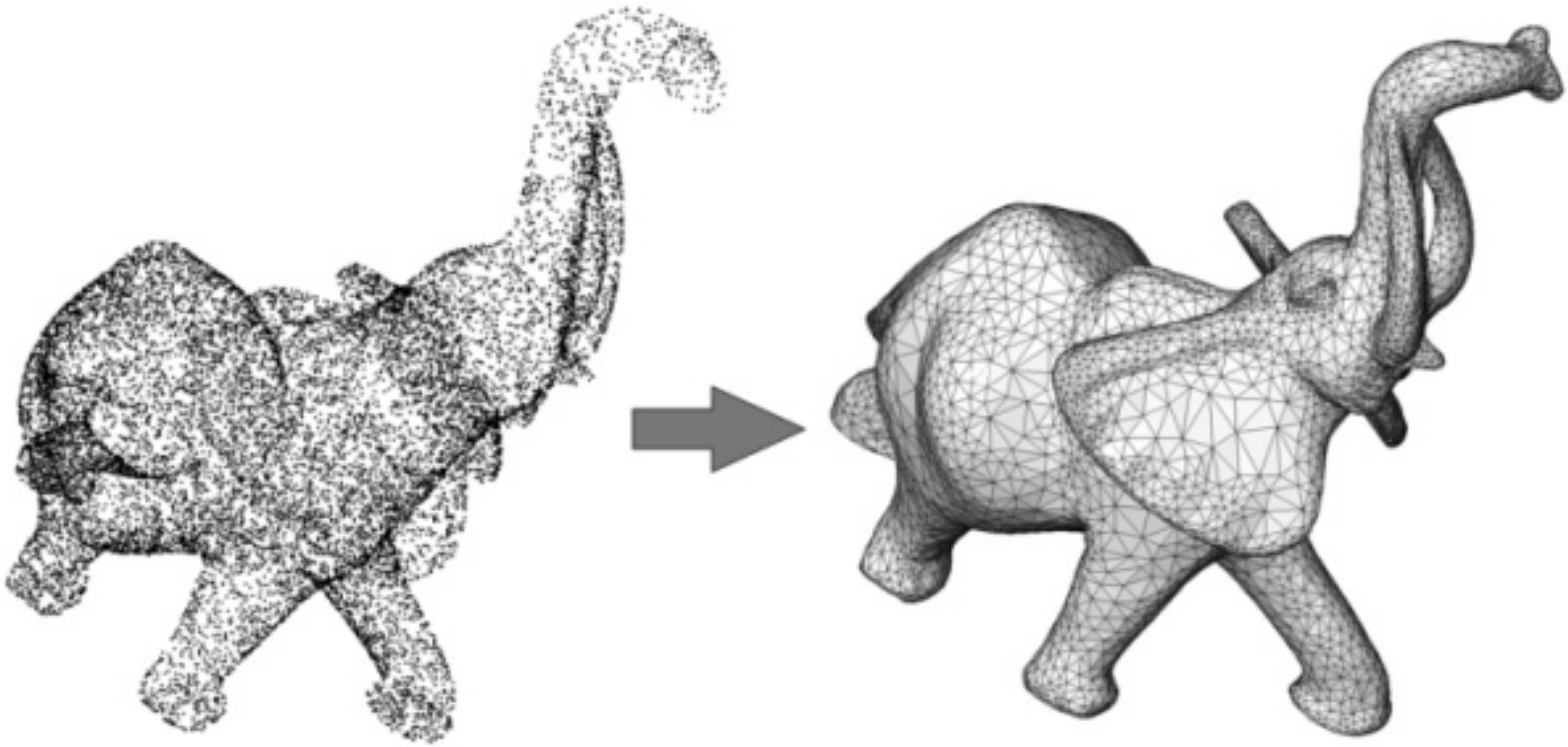


3**. Edge removal:** replace edge (c,d) by single vertex m, usually midpoint of c and d.




reconstruction
filtering
remeshing
shape analysis
parameterization
compression

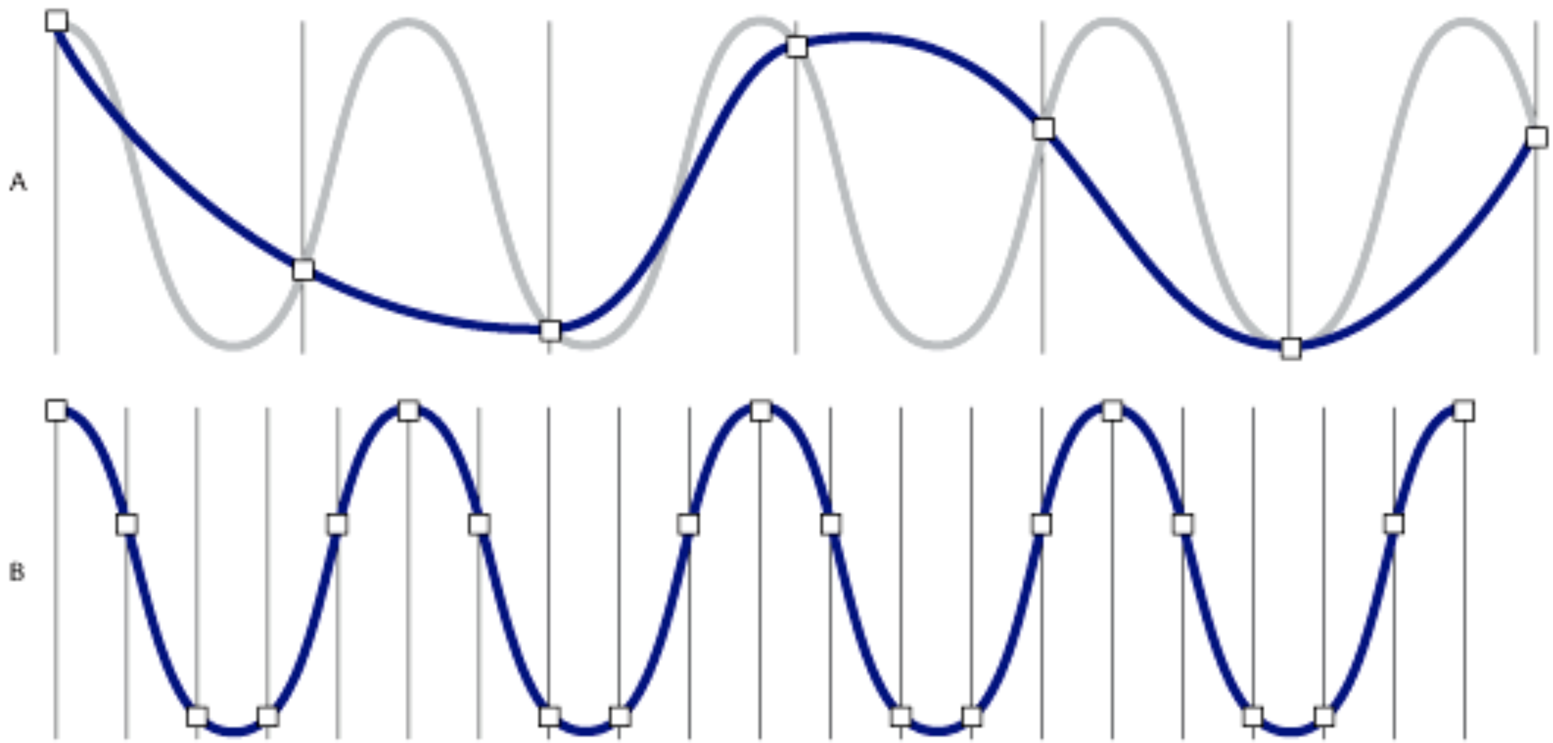
Reconstruction: *the result of a scan of an object is a set of points. The first step of any processing is to generate a surface mesh from those points.*



Remeshing as resampling

Sampling is the process of examining the value of a continuous function at regular intervals.

Note that choosing the sampling rate is not innocent:



A higher sampling rate usually allows for a better representation of the signal.

Remeshing as resampling

Surface analysis is no different from signal processing:

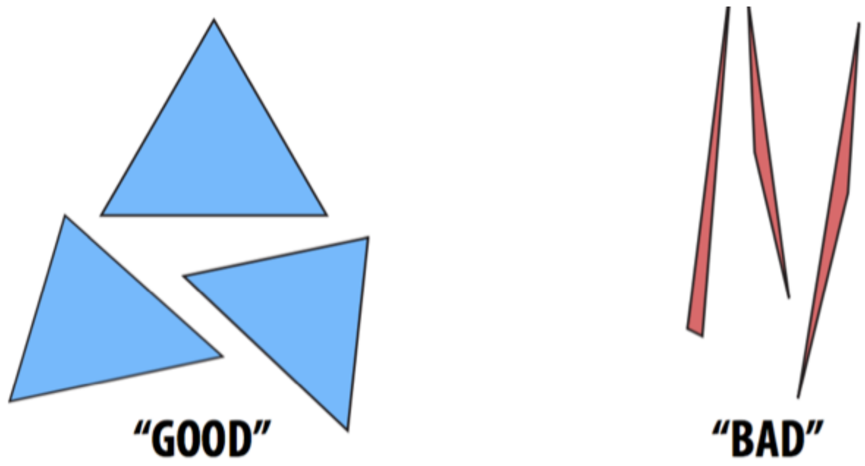
- undersampling leads to loss of features

- oversampling leads to loss of performance

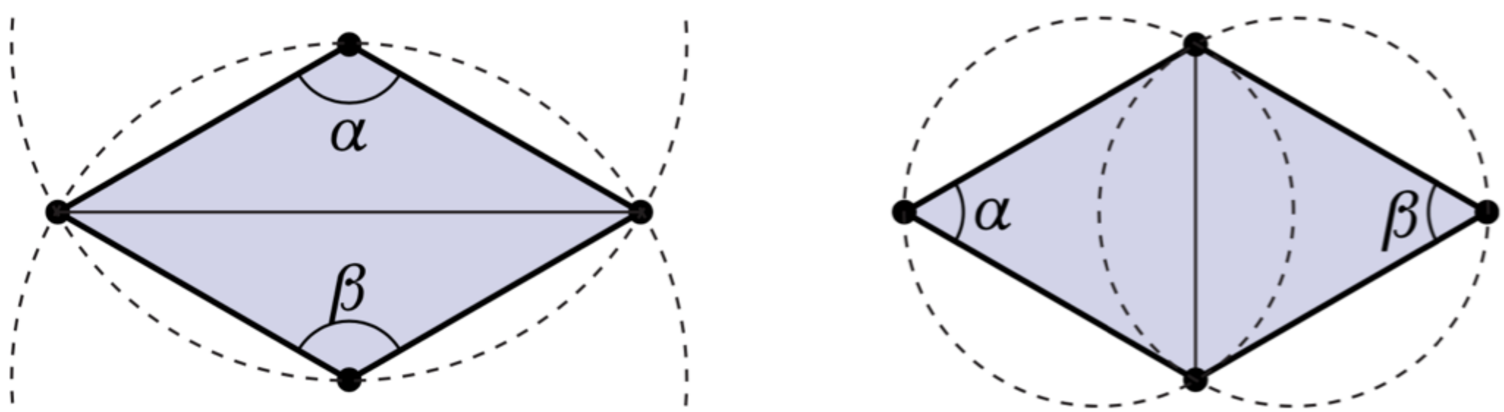
- quality sampling improves geometry and performance

Mesh “quality”

1) Triangles should be regular

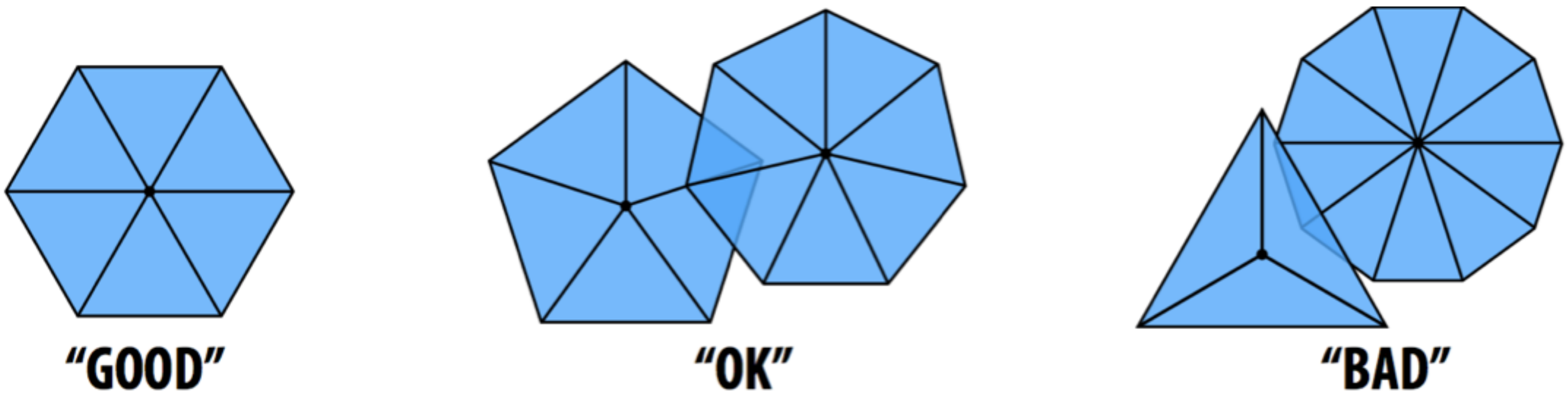


How to improve: flip edges. *When to flip? If α+β>π, flip*



Mesh “quality”

2) Vertex degree should be regular



How to improve: flips!
When to flip an edge: if total variation from degree 6 decreases, flip.