

Machine Learning and Optimal Transport for shape parametrisation

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1a) Generative Models

The first line of research consists in studying **generative models** for shape optimization of complex geometries with a large number of parameters; the objective is also to reduce the number of relevant geometrical parameters, for example for modeling naval hulls, and creating new artificial geometries similar to real data, as there are non-generative techniques for creating new real geometries (see the package PyGem [1] developed here at Sissa) but using them can be costly.

1b) Optimal transport

In the second line **semidiscrete optimal transport** is used to obtain an optimal transport map to find some intermediate geometries with some regularity constraints. An application is design optimization, in which the quantity of material for similar models must be the same.

2) Optimal transport map

Given Ω a Borel set and two measures μ and ν on Ω such that $\mu(\Omega) = \nu(\Omega)$, c a convex function $T : \Omega \rightarrow \Omega$ such that

$$\begin{cases} \nu(X) = \mu(T^{-1}(X)) & \text{for any Borel (i.e. measurable) subset } X \text{ of } \Omega \\ \int_{\Omega} c(x, T(x)) d\mu & \text{is minimal} \end{cases}$$

is called the **optimal transport** map from μ to ν . We are interested in μ continuous and ν discrete. In this case we talk of Semi Discrete Optimal Transport.

We can approximate the optimal transport map with the following algorithm:

Algorithm 1: Semi Discrete Optimal Transport [2]

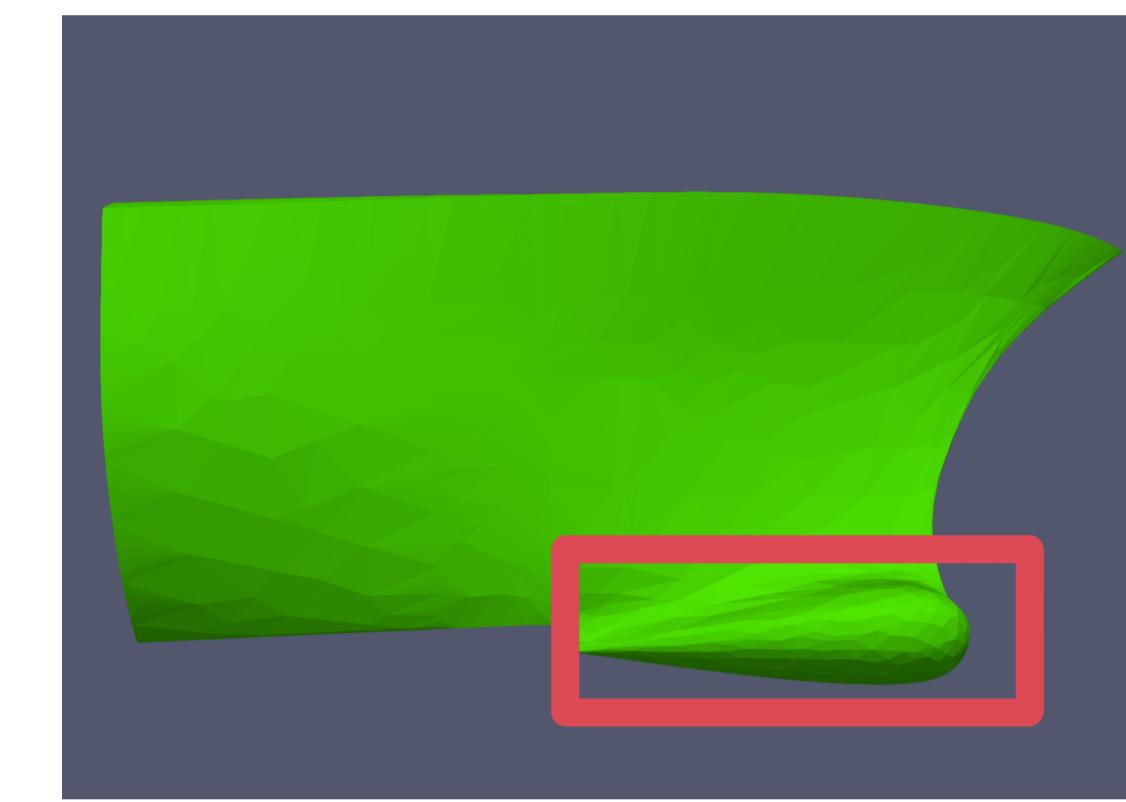
- Input:** Two tetrahedral meshes M and M' , and k the desired number of vertices in the result
- Output:** A tetrahedral mesh G with k vertices and a pair of points p_i^0 and p_i^1 attached to each vertex. Transport is parameterized by time $t \in [0, 1]$ with $p_i(t) = (1-t)p_i^0 + tp_i^1$
- 1 Sample M' with a set Y of k points
 - 2 Compute the weight vector W that realizes the optimal transport between M and Y
 - 3 Construct $E = \text{Del}(Y)$ where Del is the Delaunay Triangulation.
 - 4 For each $i \in [1 \dots k]$, $(p_i)^0 \leftarrow \text{centroid}(\text{Pow}_W(y_i) \cap M)$, $(p_i)^1 \leftarrow y_i$
 - 5 G will be the mesh defined by the topology of E with the pair of points $(p_i)^0, (p_i)^1$.

It can be proven that the linear map does not clash particles.

We modified the map to be

$$\phi_{MM'}(t) = \text{Vol}(M)^{\frac{1}{3}} \frac{tM' + (1-t)M}{\text{Vol}(tM' + (1-t)M)^{\frac{1}{3}}}$$

in order to preserve volume in intermediate times.



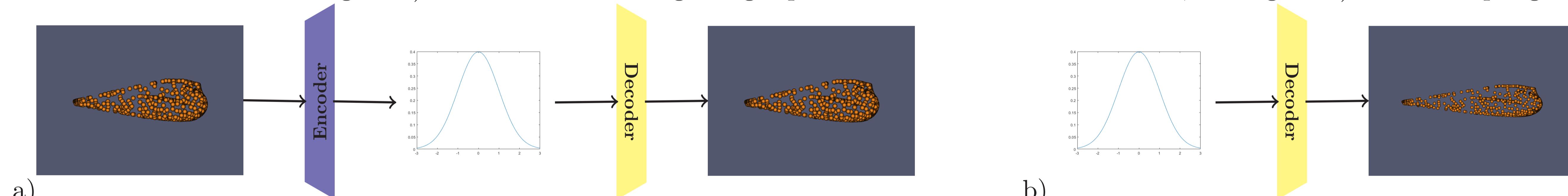
Evidenced in the red square there is the bulb, to which we applied optimal transport (using the library Geogram [4], which is currently the state of the art for semidiscrete optimal transport) with one of its deformation, as the following figure show: the first and the last figure are the bulb and its deformation respectively, in the middle there is the intermediate mesh at time $t = \frac{1}{2}$.



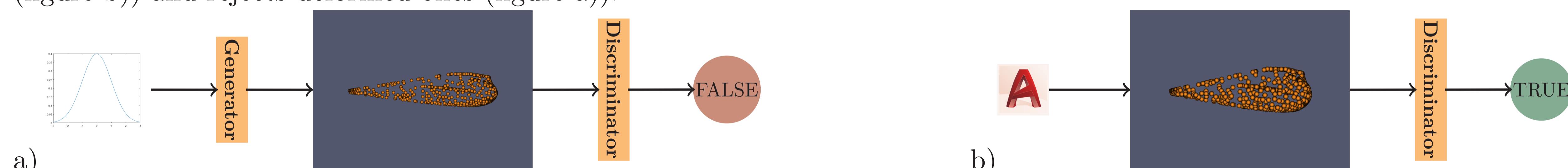
3) Generative Models

Two main model classes:

- Variational autoencoders: figure a) describes the training using a point cloud mesh of Bulbous bow, and figure b) shows sampling of a deformed Bulbous.



- Generative adversarial networks: it is characterized by a generator that samples point cloud mesh of deformed Bulbous bow and by a discriminator that accepts real Bulbous (figure b)) and rejects deformed ones (figure a)).



The loss for the discriminator is $\mathcal{L}_{\text{D}}^{\text{GAN}} = -\mathbb{E}_{x \sim p_d}[\log(D(x))] - \mathbb{E}_{\hat{x} \sim p_g}[\log(1 - D(\hat{x}))]$ and the one for the generator is $\mathcal{L}_{\text{G}}^{\text{GAN}} = \mathbb{E}_{\hat{x} \sim p_g}[\log(1 - D(\hat{x}))]$.

5 - Preliminary results and future work

Summary of our results:

- We are able to do volume preserving continuous deformation between two bulbous bows meshes using semidiscrete optimal transport. Our next step is to generalize it for more than two meshes.
- We are able to sample bulbous bows meshes using Variational Autoencoders. However, the space Z is too much sparse, so we started studying Generative Adversarial Networks.

Bibliography and Software References

- [1] Pygem, <https://github.com/mathLab/PyGeM>
- [2] A numerical algorithm for L_2 semi-discrete optimal transport in 3D, Bruno Levy, 1409.1279, 2014
- [3] Variational Autoencoders for Deforming 3D Mesh Models, Qingyang Tan, arXiv:1709.04307 ,2018
- [4] Geogram, <http://alice.loria.fr/software/geogram/doc/html/index.html>