Machine Learning and Optimal Transport for shape parametrisation

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1a) Semi-discrete Optimal transport

In the first line of research **semi-discrete 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.

1b) Generative Models of deformated geometries

The second line 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.

2) Geometry deformation with weighted barycenters in Wasserstein spaces

Given $\Omega \subseteq \mathbb{R}^n$ a Borel set and two measures μ and ν on Ω such that $\mu(\Omega) = \nu(\Omega)$, $c; \Omega \times \Omega \to \mathbb{R}^+$ a convex distance function then $\exists\, T : \Omega \to \Omega$ such that

$$\nu(X) = \mu(T^{-1}(X)) \quad \text{for any Borel subset } X \text{ of } \Omega \text{ and } \int_\Omega c(x, T(x))d\mu \quad \text{is minimal}$$

and is called the **optimal transport** map from μ to ν. We are interested in μ continuos and ν discrete. It 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 $p_i(t) = (1-t)p_i^0 + tp_i^1$

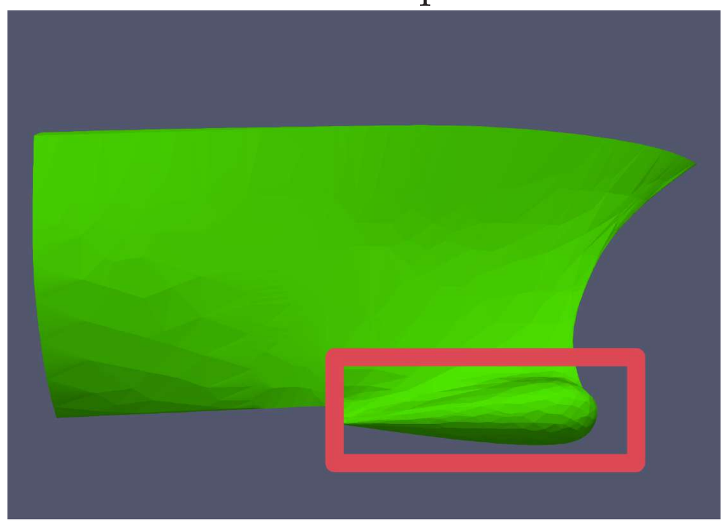
1. Sample M' with a set Y of k points
2. Compute the weight vector W that realizes the optimal transport between M and Y
3. Construct $E = Del(Y)$ where Del it the Delaunay Triangulation.
4. For each $i \in [1 \dots k]$, $(p_i)^0 \leftarrow \text{centroid}\left(\text{Pow}_W(y_i) \cap M\right)$, $\quad (p_i)^1 \leftarrow y_i$
5. G will be the mesh defined by the topology of E with the pair of points $(p_i)^0$,$(p_i)^1$.

We modified the map to be

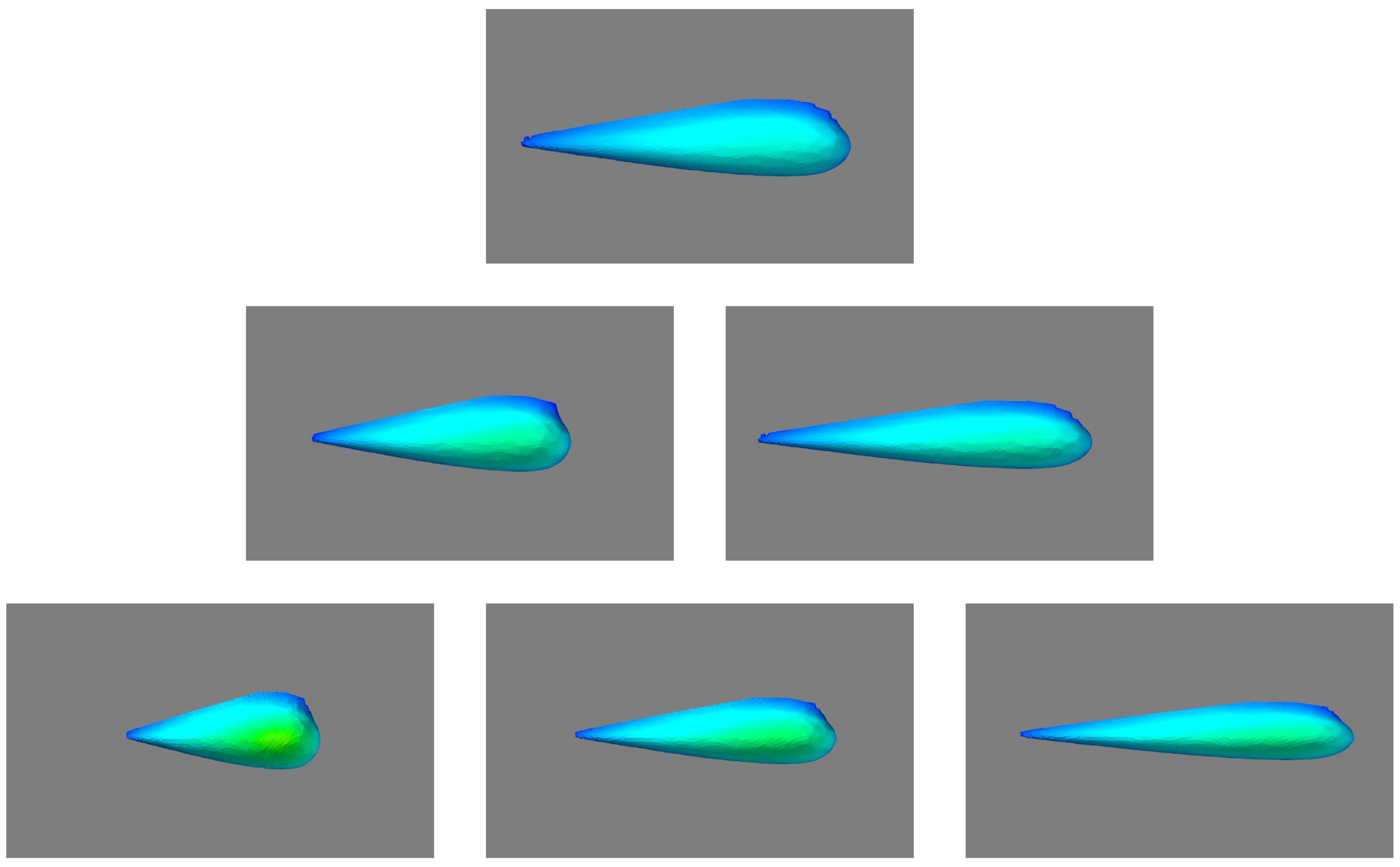
$$\phi_{MM'}(t) = Vol(M)^{\frac{1}{3}} \frac{tM' + (1-t)M}{Vol(tM' + (1-t)M)^{\frac{1}{3}}}$$

in order to preserve volume in intermediate times.

Let's now show a ship hull.



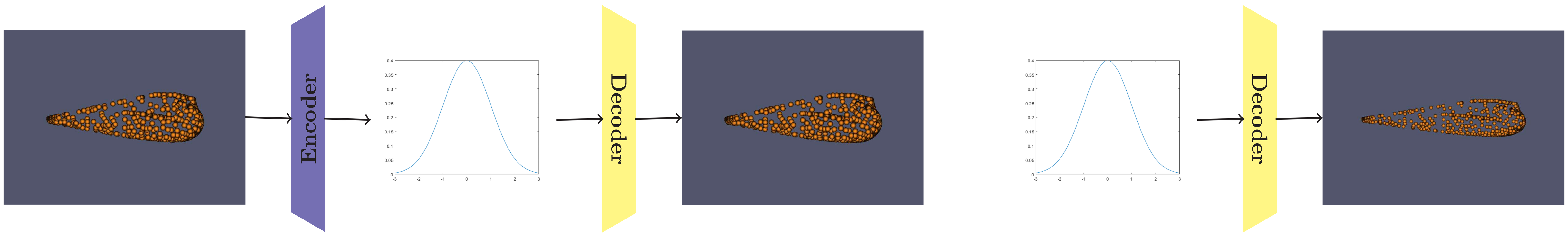
Highlighted in the red square there is the bulb, to which we applied semi-discrete optimal transport to a bulb (using the library Geogram [4], which is currently the state of the art for semidiscrete optimal transport) with two of it's deformations: the figures at the edges are the bulb and its deformation respectively, in the middle there are the intermediate meshes at time $t = \frac{1}{2}$.



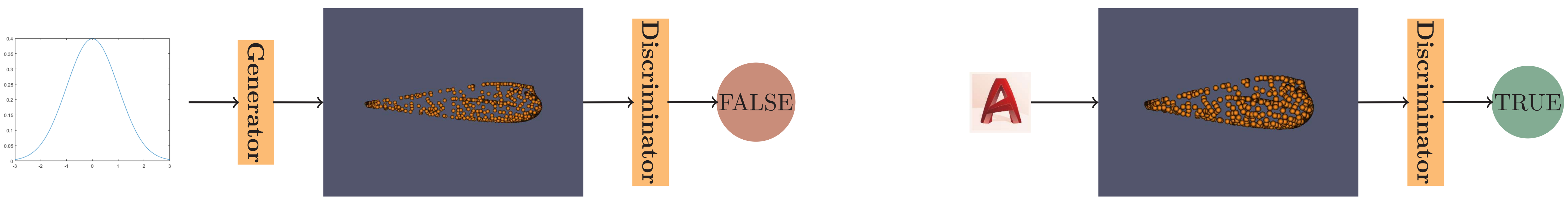
2b) Generative models for reduction in parameter space

Two main model classes:

- Variational autoencoders(VAE): the figure describes the training using a point cloud mesh of Bulbous bow, and the right figure 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 (right figure)) and rejects deformed ones (left figure)).



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

5 - Preliminary results and future work

- We are able to do volume preserving continuos deformation between two bulbous bows meshes using semidiscrete optimal trasport. Our next step is to generalize it for more complex geometries, and apply it shape optimization and reduced order modelling.
- 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`