Machine Learning and Optimal Transport for shape parametrisation

Guglielmo Padula, Francesco Romor, Giovanni Stabile, Nicola Demo, Gianluigi Rozza
Mathematics Area, mathLab, SISSA, International School of Advanced Studies, Trieste, Italy

Introduction

- generative models of shape optimization for complex geometries with an elevated number of parameters; the objective is to learn the shape using a minor number of parameters, for example for modeling naval hull, and creating new geometries similar to real data, as creating new geometries can be costly.
- Semidiscrete Optimal transport is used to obtain an optimal transport map to find some intermediate geometries with some regularity constraints. We show results regarding Variational Autoencoders, Semi-Discrete Optimal Transport applied to simple geometries. The extension of Semi Discrete Optimal Transport to three meshes will also be discussed.

1 - Volume of a Tetrahedral Mesh

Consider a tetrahedal mesh M composed of N tetrahedras. Let M_i the i-th tetrahedra of M and $a^{(i)}, b^{(i)}, c^{(i)}, d^{(i)}$ it's edges represented as column vectors of $\mathbb{R}^3$. It can be proven that $Vol(M_i) = \frac{|det(A_i)|}{6}$ where A_i is the matrix $[a^{(i)} - d^{(i)} \quad b^{(i)} - d^{(i)} \quad c^{(i)} - d^{(i)}]$.

It follows that

$$Vol(M) = \sum_{i=1}^{N} Vol(M_i) = \sum_{i=1}^{N} \frac{|det(A_i)|}{6}$$

2 - Optimal Transport

Given Ω a Borel set and two measures μ and ν on Ω such that $\mu(\Omega) = \nu(\Omega)$, c a convex function $T : \Omega \to \Omega$ 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 continuos and ν discrete. It this case we talk of Semi Discrete Optimal Transport.
The power diagram $\mathrm{Pow}_W(p_i)_W(P)$ is the partition of $\mathbb{R}^d$ into the subsets $\mathrm{Pow}_W(p_i) := \left\{ x \mid \|x - p_i\|^2 - w_i < \|x - p_j\|^2 - w_j \quad \forall j \neq i \right\}$.
The map T_W defined by $\forall i, \forall p \in \mathrm{Pow}_W(p_i), T_W(p) = p_i$ is called the assignment defined by the power diagram $\mathrm{Pow}_W(P)$ and is an optimal transport map.
Knowing this, we can approximate the optimal transport map with the following algorithm:

Data: Two tetrahedral meshes M and M', and k the desired number of vertices in the result
Result: 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 $i \in [1 \dots k], (p_i)^0 \leftarrow \mathrm{centroid}(\mathrm{Pow}_W(y_i) \cap M), \quad (p_i)^1 \leftarrow y_i$
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. This algorithm is implemented in the library Geogram created by Bruno Levy.

3a - Extension of Optimal Transport: volume preserviness in intermediate times

Let $M^{(0)}$ and $M^{(1)}$ the results of the Optimal Transport. In theory, $M^{(0)} \neq M$ because of the intersection with the power diagram so $M^{(0)} \neq M$. For similar reasoning, $M^{(1)} \neq M'$. However, with k large, it can be shown experimentally that the meshes are similar. Let us suppose we are in this case and so $Vol(M^{(0)}) = Vol(M^{(1)})$. As the volume of a mesh is a scaled sum of determinant and determinant are non linear functions, in general, we have $Vol(tM^{(0)} + (1-t)M^{(1)}) \neq Vol(M^{(0)})$ so a simple linear map cannot preserve volumes in intermediate times. Let $M_i^{(0)}$ and $M_i^{(1)}$, $A_i^{(0)}$ and $A_i^{(1)}$ like in section 1. From the property that the linear map does not clash particles, we have that $det(A_i^{(0)})det(A_i^{(1)}) > 0 \forall i \in 1 \dots N$. Otherwise, as determinant is a continuous function, we would have that $\exists t^*$ s.t $0 = det(t^* A_i^{(0)} + (1-t^*)A_i^{(1)}) = 6 * Vol(t^* M_i^{(0)} + (1-t^*)M_i^{(1)})$ so a tetrahedra disappear and this cannot happen because of the non clashing particles property. So we can cut the absolute value out and obtain $Vol(tM^{(0)} + (1-t)M^{(1)}) = \sum_{i=1}^{N} Vol(tA_i^{(0)} + (1-t)A_i^{(1)}) = \sum_{i=1}^{N} \frac{Det(tA_i^{(0)} + (1-t)A_i^{(1)})}{6}$.
The volume in this case is just a third grade polynomial of grade 3, and can also be calculated analitycally knowing $M^{(0)}$ and $M^{(1)}$. With this motivations, we define another map for optimal transport

$$\phi_{M^{(0)}M^{(1)}}(t) = Vol(M^{(0)})^{\frac{1}{3}} \frac{tM^{(1)} + (1-t)M^{(0)}}{Vol(tM^{(1)} + (1-t)M^{(0)})^{\frac{1}{3}}}$$

This map is an optimal transport map as $\phi_{M^{(0)}M^{(1)}}(0) = M^{(0)}$ and $\phi_{M^{(0)}M^{(1)}}(1) = M^{(1)}$ and preserves volume in intermediate times by definition.

3b - Extension of Optimal Transport: extension to three meshes

Let M, M', M'' three meshes. Let us suppose we calculate the OTM from M to M' and from M'' selecting M' to be sampled in the same way in both transports, so the resulting mesh will be the same (because in the algorithm does not depend on the other). So let $M^{(0)}$, $M^{(1)}$ and $M^{(2)}$ the approximation of M, M', M'' respectively. So with the same assumption as before we can define a new transport map

$$\phi_{M^{(0)}M^{(1)}M^{(2)}}(t) = \begin{cases} Vol(M^{(1)})^{\frac{1}{3}} \frac{2tM^{(1)} + (1-2t)M^{(0)}}{Vol(2tM^{(1)} + (1-2t)M^{(0)})^{\frac{1}{3}}} & 0 \le t \le \frac{1}{2} \\ Vol(M^{(1)})^{\frac{1}{3}} \frac{(2t-1)M^{(2)} + (2-2t)M^{(1)}}{Vol((2t-1)M^{(2)} + (2-2t)M^{(1)})^{\frac{1}{3}}} & \frac{1}{2} \le t \le 1 \end{cases}$$

that goes from $M^{(0)}$ to $M^{(1)}$ and then from $M^{(1)}$ to $M^{(2)}$.

4 - Variational Autoencoder

A Variational Autoencoder is a neural network composed of two main components, an encoder $E : X \to Z$ and a decoder $D : Z \to X$ where usually $dim(Z) << dim(X)$. If it is possible to sample from Z after E and D are trained it is possible to sample from X by sampling from Z and applying D. Z is also useful for dimensionality reduction.

5 - Preliminary results and future work

Summary of our results:

- We are able to do volume preserving deformation between three meshes using Optimal Trasport Map with meshes of convex polyhedras, our next step is to generalize it for more than three meshes, which is nontrivial (as M_0 and M_2 are nonsampled), and also to test less regular meshes.
- We are able to sample parallelepipeds centered in 0 with volume 1. However, the space Z is too much sparse even for these simple meshes, so we are planning to move to Generative Adversarial Networks.

Bibliography and Software References

- Geogram, `http://alice.loria.fr/software/geogram/doc/html/index.html`