

Generative models for shape parametrization

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General Objective

The general objective of our research is, given a set of 3D meshes generated by complex methods with a large number of parameters, to find a generative model such that:

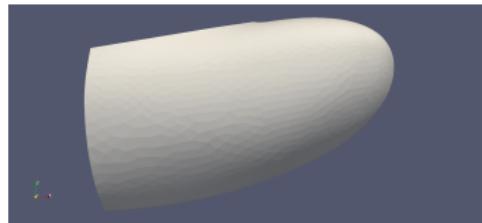
- Reduces the number of effective parameters via dimensionality reduction
- Sampling (and if possible training) using this method should be fast as possible
- Generated samples should satisfy some **convex** equality and/or inequality constraint
- (**Optional**) the distribution of useful quantities associated to the object should be similar between the generated samples and the real samples.

Motivation

- Complex methods are very computationally complex (the data generated in the code uses VFFD which is fast, however there are methods based on differential equations that take days to complete)
- A possible application are inverse problems with non convex constraints, which require exhaustive search, they would scale exponentially in the number of parameters.
- Ideally we would like to run simulation on this samples, and indeed to get not this simulations to explode, we need some convex constraints on the output.

Data

We focus on the problem of deforming a naval hull bulb. The data is obtained by deforming using Volume Preserving FFD with 27 parameters, which deforms object by moving control points and preserves the volume. We want volume preservation because it is a nice property in simulations. It can be rewritten as a sequence of linear constraints. As we want to focus only on the bulb, we first take only one half of the ship, and then we do two cuts to obtain the bulb. The ship is a triangular mesh so it has an internal topology.



The generative models

Our generative model should not touch the points on the boundary and move the points on the symmetry plane only horizontally. It should also preserve volume exactly. For this reason we need to heavily customize classic generative models and we split the data in two parts, a part (x) that will consist in the points that don't belong to the symmetry plane and a part y that belong to the symmetry plane. We use:

- Vanilla Autoencoder
- β Variational Autoencoder
- Boundary Equilibrium GAN
- Adversarial Autoencoder

All this models require an Encoder and a Decoder, whose architectures will be the same in every model. All models are trained using AdamW.

Long life to the LBR

Our basic layer (which we call LBR) is formed with:

- A linear Layer
- A BatchNorm1D Layer
- A ReLU Layer
- A Dropout Layer

Custom Layers

We also use a series of custom layer to improve the training and the sampling:

- A PCA Layer
- A smoothing Layer
- A volume normalization Layer

These layers are not strictly necessary to obtain decent samples in the generation phase (the network learns to preserve volume even without the layer), however the sample quality is greatly increased with the use of this layers.

PCA Layer

We use PCA to reduce the initial dimensionality of the data, which will consist in two layers: a PCATranformLayer and a PCAInverseTransformLayer. Note that PCA does not compress data as the relative reconstruction error is very low (around 10^{-8}).

Smoothing Layer

This is a layer that applies laplacian smoothing

$$P_i = \frac{1}{|N_i|} \sum_{j \in N_i} P_j$$

where N_i are the neighbours of index i . Note that the laplacian smoother is applied only to points that are not on the boundary and not on the symmetry plane.

Volume Normalization

The Volume Normalization layer solves the optimization problem of finding the lowest variation of the points such that the volume is constant and such that the points don't clash with the boundary. This layer is well behaved because both the constraints are linear and so the solution is unique. Notice that because the problem is quadratic programming problem, a solution is found very quickly and so it does not slow the training.

Encoder

The Encoder takes as input x and y and applies for x :

- A PCATransform from the dimension of x (around 700) to 24.
- A LBR from 24 to 500
- A series of LBR with hidden dim 500
- A final LBR from 500 to the latent space of x which has dimension 11 (estimated with TwoNN).
- The output is standardized.

The same is done with y (original dimension around 200, latent space 1, hidden dim 500).

Decoder

The Decoder takes as input the z of size 11 and w of size and applies for z :

- An LBR from 11 to 500
- A series of LBR with hidden dim 500
- A final LBR from 500 to the latent space of 24
- Then PCAInverseTransform is applied

The same is done with w . Then the two outputs are concatenated and

- Smoother is applied
- VolumeNormalizer is applied

Vanilla Autoencoder

This is a classic autoencoder, customized for having two inputs and two outputs.

$$z, w = Enc(x, y)$$

$$\hat{x}, \hat{y} = Dec(z, w)$$

$$Loss = \frac{1}{2} (||x - \hat{x}||_2^2 + ||y - \hat{y}||_2^2)$$

Sampling is done by sampling from $Normal(0, 1)$ and then by applying the Decoder. This brings useful results because of the standardization in the Encoder.

β Variational Autoencoder I

$$\mu_1, \mu_2 = Enc(x, y)$$

$$\sigma_1 = LBR(\mu_1)$$

$$\sigma_2 = LBR(\mu_2)$$

$$z \sim Normal(\mu_1, \sigma_1)$$

$$w \sim Normal(\mu_2, \sigma_2)$$

$$\hat{x}, \hat{y} = Dec(z, w)$$

$$A = Normal(\hat{x}, \sigma)$$

$$B = Normal(\hat{y}, \sigma)$$

where σ is a network parameter.

β Variational Autoencoder II

$$Loss = \frac{1}{2}(p_A(x)) + p_B(y)) +$$

$$\frac{\beta}{2}(KL(Normal(0, 1) | Normal(\mu_1, \sigma_1)) + KL(Normal(0, 1) | Normal(\mu_2, \sigma_2)))$$

β VAE's are VAE's with an additional hyperparameter β in the loss function for avoid model collapse or to enforce a better prior posterior matching depending on the situation (in this case we use it for the first reason). Sampling is done by sampling from $Normal(0, 1)$ and then by applying the Decoder. Note that this is not the usual way in which sampling is done. This is necessary to ensure volume preservation.

Boundary Equilibrium GAN

A Boundary Equilibrium GAN is composed by a Generator (which has a Decoder architecture) and by an AutoEncoder which is used as discriminator.

$$z_d, w_d = AE.encoder(x, y)$$

$$z_g \sim Normal(0, 1)$$

$$w_g \sim Normal(0, 1)$$

$$x_g, y_g = Gen(z_g, w_g)$$

$$\hat{x}, \hat{y} = AE.decoder(z_d, w_d)$$

$$\hat{x}_g, \hat{y}_g = AE(x_g, y_g)$$

$$Loss_{AE} = \frac{1}{2}(||x - \hat{x}||_2^2 + ||y - \hat{y}||_2^2) - k_t \frac{1}{2}(||x_g - \hat{x}_g||_2^2 + ||y_g - \hat{y}_g||_2^2)$$

$$Loss_{Gen} = \frac{1}{2}(||x_g - \hat{x}_g||_2^2 + ||y_g - \hat{y}_g||_2^2)$$

$$k_t = k_{t+1} + \lambda_t [\gamma \frac{1}{2}(||x - \hat{x}||_2^2 + ||y - \hat{y}||_2^2) - \frac{1}{2}(||x_g - \hat{x}_g||_2^2 + ||y_g - \hat{y}_g||_2^2)]$$

Latent Discriminator

For the next and last model, we need a discriminator that acts on the latent space. For z is composed by:

- A series of LBR from latent to latent
- A LBR from latent to 1

Same for w .

Then it takes the sum of the two results.

Adversarial Autoencoder

It is an intersection between a AutoEncoder and a Gan. It is composed by a Encoder, a Decoder and a Discriminator.

$$z, w = \text{Decoder}(x, y)$$

$$\hat{x}, \hat{y} = \text{Decoder}(z, w)$$

$$z_g \sim \text{Normal}(0, 1)$$

$$w_g \sim \text{Normal}(0, 1)$$

$$\text{Loss}_{AE} = \frac{1}{2} (||\hat{x} - x||_2^2 + ||\hat{y} - y||_2^2) - D(z, w)$$

$$\text{Loss}_D = D(z, w) - D(z_g, w_g)$$

Notice that, in this case the Generator is the Decoder and that real and fake data are inverted with respect to usual GAN's.

Maximum Mean Discrepancy

The quantity

$$\begin{aligned} MMD(P, Q) = & (\mathbb{E}_{X, X' \sim P} k(X, X') + \mathbb{E}_{Y, Y' \sim Q} k(Y, Y')) \\ & - 2\mathbb{E}_{X \sim P, Y \sim Q} k(X, Y))^{\frac{1}{2}} \end{aligned}$$

where k is a kernel, is called Maximum Mean Discrepancy.

Theorem

If k is Gaussian, then $MMD(P, Q) = 0 \Leftrightarrow P = Q$.

Now let's define

$$RelMMD(P, Q) = \frac{MMD(P, Q)}{(\mathbb{E}_{X, X' \sim P} k(X, X') + \mathbb{E}_{Y, Y' \sim Q} k(Y, Y'))^{\frac{1}{2}}}$$

which is scaled between 0 and 1.

Evaluation

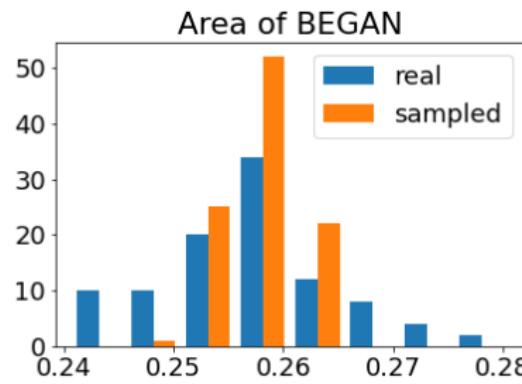
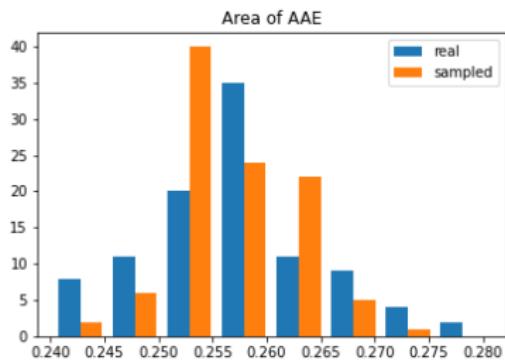
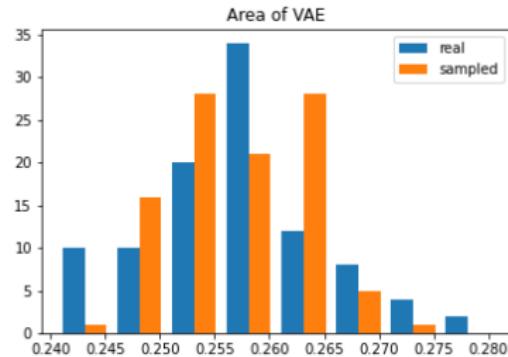
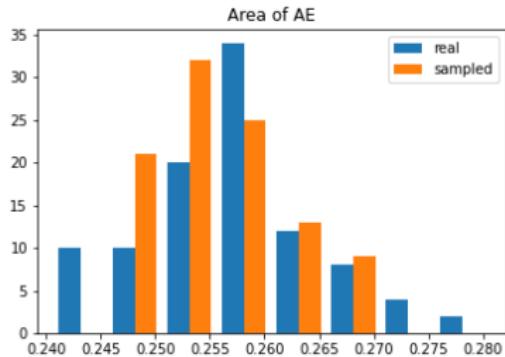
We use the following metrics:

- Relative Reconstruction Error
- RelMMD between data and samples
- RelMMD between the areas of data and samples
- RelMMD between the gaussian curvatures of data and samples
- Variance of the samples

Results

	AE	AAE	VAE	BEGAN
$RelMMD(Area)$	0.011	0.012	0.017	0.014
$E[\min_X \frac{\ Dec(Z) - X\ }{\ X\ }]$	0.01	0.01	0.009	0.01
$Var(Dec(Z))$	0.024	0.027	0.017	0.018
$RelMMD(GC)$	0.17	0.18	0.19	0.20
$RelMMD(Id)$	0.016	0.016	0.018	0.019

Area



Total Curvature

