CentraleSupélec

Pôle projet 05 - Formation à la recherce

Tsunami propagation using neural networks

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Contents

Chapter 1 - Introduction

1.1 Context and objectifs

Tsunamis do not occur very often but are devastating phenomena. Research and studies about tsunamis try to predict the impact of such events to protect people. Due to the sheer scale of tsunami, laboratory and analytical models are not relevant. The former because we can not obtain an equivalent scale model in a lab, the latter because there is no analytical solution to the propagation equations. Although a numerical resolution can approximate the solution, it requires a huge computing power and time without taking into account the accuracy errors due to turbulence phenomena.

1.2 State of the art

1.3 Contribution

1.4 Report Structure

First, it is presented how important and effective this approach is, then the second chapter shows basic concepts about a neural network and its behavior, as well as a brief introduction to differential equations. Then in the third paragraph we explain our approche and solve some partial differential equations using neural networks. After that, in the fifth paragraph, the describes how obtain the domain to do the Tsunami simulation, that is, the mesh to make the simulation.

Chapter 2 - Concepts

2.1 Neural networks

Now the basis of multiple state of the art technologies in data science, neural networks provide a framework we hope can solve propagation equations in a shorter time than with regular finite elements.
For now, we will focus on the study of multilayer perceptron, one of the first neural networks to have been developped. They consist in an input layer, a vector of n components, and an output layer, of p components. The input is subjected to a series of linear operations and non-linear activations are applied trough "hidden layers" to get the output.
A multilayer perceptron can then be seen as a non linear function:

$$\mathcal{N} : \mathbb{K}^n \to \mathbb{K}^p$$

If we note g_i the (non-linear) activation function, and W_i and b_i the weight and bias matrix of the ith hidden layer, then, for a MP with k hidden layers:

$$\forall x \in \mathbb{K}^n, \mathcal{N}(x) = g_k(b_k + W_k g_{k-1}(b_{k-1} + W_{k-1} g_{k-2}(\dots(b_1 + W_1 x)))) \tag{2.1}$$

Through training epoch, passes through the training dataset coupled with gradient descent, we want $\mathcal{N}$ to approach a function of interest.

2.2 Partial Differential Equation

Our goal is to solve the propagation equation of a tsunami, which is a partial differential equation (PDE). In a general sense, a PDE is defined as:

$$(E) : \begin{cases} \mathcal{Q}(u, \nabla u, Hu, \dots)(x) = 0 & \text{inside } \Omega \\ \mathcal{R}(u, \nabla u, Hu, \dots)(x) = f(x) & \text{on } \partial\Omega \end{cases}$$

Where $\mathcal{Q}$ and $\mathcal{R}$ are linear operators, Ω is the domain considered,
and $u : \mathbb{K}^n \to \mathbb{K}^p$ is the solution to (E).

Our goal is to replace u with a neural network $\mathcal{N}$ and train it to get a solution to (E). However, this would mean training on both the domain and its boundary. To avoid this case as the boundary is always defined with boundary conditions, we reformulate the problem:

Instead we replace u with Ψ defined as:

$$\Psi(x) = A(x) + F(x)\mathcal{N}(x) \tag{2.2}$$

Where A verifies the boundary conditions, and F is null on the boundary.
As such, we unconstrained the problem, and the neural network can train inside the domain, with the boundary conditions handled by the above mentionned functions.

2.3 Find A

In this section we propose two choices for the function A in 2 different contexts.
Let K be a point in space with coordinates $\vec{x_K} = \sum x_j \vec{e_j}$

2.3.1 Function 1

$$\forall x \in \mathbb{R}^k, \psi_K(x) = \begin{Bmatrix} \exp\left(-\frac{1}{l^2 - d(x,K)^2}\right) & if\ d(x,K)^2 < l^2 \\ 0 & else \end{Bmatrix}$$

Where $d(x,K)^2 = \|x - x_K\|^2$
This function has the advantage of not interacting with the space located beyond a distance l away from point A

Use in our case

Let Ω be a domain, and $\partial\Omega$ its boundary. We sample N points from the boundary with coordinates x_i such as $g(x_i) = g_i$. Let us use

$$l = \min_{1 \leq i,j \leq N} \|x_i - x_j\|$$

Then, we can use the following function to compute the value of the boundary with interesting properties.

$$\Psi(x) = \exp\left(\frac{1}{l^2}\right) \sum_{i=1}^{N} g_i \psi_i(x)$$

Boundary conditions

We do verify the boundary conditions:

$$If\ x = x_j \in \partial\Omega, \Psi(x_j) = g_j$$

As by hypothesis, for ψ_j the distance is null, and for all other ψ_i we are at a distance greater than l away from x_i.

Regularity

By summing ψ functions, we have that Ψ is a class C^∞ function.

Derivative

By using chain rule, we can easily calculate the derivative according to any variable j with

$$\partial_j \Psi(x) = \exp\left(\frac{1}{l^2}\right) \sum_{i=1}^{N} g_i \partial_j \psi_i(x)$$

and

$$\partial_j \psi_i(x) = \frac{-2(x_j - x_{Aj})}{(l^2 - d(x,i)^2)^2} \psi_i(x)$$

Bounded function

By definition, we have

$$\forall x \in \mathbb{R}^k, \min_{1 \leq i \leq N} g_i \leq \Psi(x) \leq \max_{1 \leq i \leq N} g_i$$

Ease of computation

To calculate Ψ and its gradient, a lot of elements are redundant and thus can be evualated once, like l (when we sample the boundary) and $l^2 - d(x,i)^2$ for each point of the boundary.

Issues

This function is too restrictive to be usable in practice. With too much sample boundary points, this function becomes a series of spikes, and thus does not approximate the boundary asymptotically. In case of a small amount of samples, this function is useful.

2.3.2 Function 2

$$\forall x \in \mathbb{R}^k, \psi_K(x) = 1 - \tanh\left(\frac{d(x,K)}{l}\right)^2$$

This time with:

$$\Psi(x) = 0.5 \sum_{i=1}^{N} g_i \psi_i(x)$$

This time, our function verifies the boundary conditions only asymptotically with a uniformly sampled boundary.
The 0.5 coefficient is their to correct for the first order interactions between two adjacent ψ_K.
Through numerical simulations, we obtain a smoothed boundary that closely ressembles the real boundary with enough sample points. In our simulation, this function will be mostly used as the A function.

2.4 Find F

Set $(d,n) \in \mathbb{N}^*$ and $(x_i)_{i\in[\![0;n-1]\!]} \in \mathbb{R}^d$ distinct one another. We seek a polynomial $F \in \mathbb{K}[X]$ such that $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and

$$\forall i \in [\![1;n]\!],\ F(x_i) = 0 \text{ and } \exists x_n :\ F(x_n) \neq 0$$

2.4.1 Case 1D

In the case $d = 1$, Vandermonde polynomials are a good start. The only thing to add to the construction is a point where the polynomial F is not null. Assuming the orthobarycentre of the family $(x_i)_{i\in[\![0;n-1]\!]}$ is not already inside, let's take the orthobarycentre of these points defined as $x_n := \frac{1}{n}\sum_{i=0}^{n-1} x_i$.
The system induced is this one :

$$\begin{pmatrix} 1 & x_0 & \dots & x_0^n \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n-1} & \dots & x_{n-1}^n \\ 1 & x_n & \dots & x_n^{n-1} \end{pmatrix} \begin{pmatrix} a_0 \\ \vdots \\ a_{n-1} \\ a_n \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

that one can solve thanks to the inversion of the Vandermonde matrix, which is non-singular since all the points are distinct one another thanks to the assumption.

2.4.2 Case 2D

The work done here for $d = 2$ is meant to be easily generalizable to even greater values of d. Set $\forall i \in [\![0; n-1]\!], x_i$ has as coordinates $(x_{i,0}, x_{i,1})$.

Matrix method

Start of an idea (inspired from Vandermonde matrix in 1D)

Globally, F can be defined in $\mathbb{R}_{n+1}[X]$ considering its roots $(x_i)_{i\in[\![0;n-1]\!]}$ and the point x_n where it is not null. Therefore, set x_n the orthobarycentre with the same assumption as previously and $(\alpha_{ij})_{\{(i,j)\in\mathbb{N}:i+j\leq n\}} \in \mathbb{R}^{2n}$ such that

$$\forall (x,y) \in \mathbb{R}^2,\ F(x) = \sum_{\{(i,j)\in\mathbb{N}:i+j\leq n\}} \alpha_{ij} x^i y^j$$

$$\begin{pmatrix} 1 & x_{0,0} & x_{0,1} & x_{0,0}x_{0,1} & \dots & x_{0,1}^n \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n-1,0} & x_{n-1,1} & x_{n-1,0}x_{n-1,1} & \dots & x_{n-1,1}^n \\ 1 & x_{n,0} & x_{n,1} & x_{n,0}x_{n,1} & \dots & x_{n,1}^n \end{pmatrix} \begin{pmatrix} \alpha_{00} \\ \vdots \\ \alpha_{0(n-1)} \\ \alpha_{0n} \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

Actually, Vandermonde does not give any proof of the non-singularity of the left matrix and one could thought about putting more combinations of the coordinates of each point to extract a non-singular matrix after. Yet, finding this extracted matrix remains computationally heavy in addition to being uncertain.

In hindsight

The realm this idea steps into is the realm of principal component analysis. It remains interesting considering the fast differentiation of the polynomial one could get after. Nevertheless, it could force us to already use machine learning which will require some time to compute accurately and will always remain an approximation of the true solution we seek.

Direct approach

In this kind of situation, constructing the polynomial

$$F : (x, y) \mapsto \prod_{m=0}^{n-1} (x - x_i)(y - y_i)$$

quickly comes to mind. Nevertheless, F would be to often null on the domain and could induce great errors after. So, the idea is to replace the given factor by one null only at a given point as shown here:

$$\forall (x, y) \in \mathbb{R}^2,\ F_r(x, y) = \prod_{k=0}^{n-1} ((x - x_k)^2 + (y - y_k)^2)$$

$$\forall (x, y) \in \mathbb{R}^2,\ F_c(x, y) = \prod_{k=0}^{n-1} ((x - x_k) + i(y - y_k))$$

$$\forall (x, y) \in \mathbb{R}^2,\ F_s(x, y) = \prod_{k=0}^{n-1} (\sin(x - x_k) \sin(y - y_k))$$

- $\forall (x, y) \in \mathbb{R}^2,\ F_r(x, y) = |F_c(x, y)|^2$ and $|\ F_s(x, y)| <= 1$
- the coefficients of F_c are faster to compute but harder to evaluate than the ones of F_r
- the coefficients of F_s are as fast as F_c to compute and it's bounded, a important characteristical

Chapter 3 - PDEs using neural networks

3.1 Hyperparameters

Here is the scheme of model tuning followed:

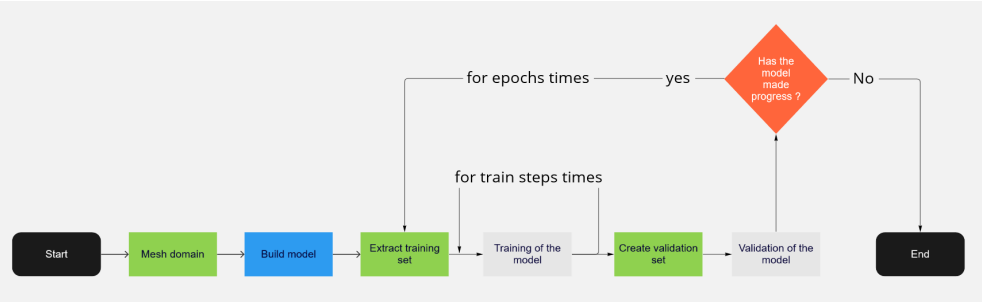


Figure 3.1: scheme of a model tuning

The red box involves using an early stopping callback to stop the epoch loop when the model begins to overfit. A `patience` integer set how far the system will go back in history. If during `patience` epochs the has not made progress the epoch loop is stopped.
The hypertuning comes when one wants to construct a model and a training that will end to a low validation error. Let's list all the hyperparameters involved in this scheme applied for the Poisson equation on a square domain:

- `grid_length`: integer setting the number of points in the domain to `grid_lengthxgrid_length`
- `l_units`: list of integers depicting the number of hidden layers and the number of neurons per layer of the sequential machine learning model
- `l_activations`: list depicting the activation functions of each layer of the model
- `noise`: integer in $\{0, 1\}$ conditioning the use of a Gaussian layer of mean 0 after the input layer
- `stddev`: the standard deviation of the Gaussian layer when it is used
- `optimizer`: string depicting the optimizer used
- `learning_rate`: float setting the learning rate of the previous optimizer
- `epochs_max`: integer setting the number of maximum epoch loops
- `n_trains`: integer setting the number of train loops
- `batch_size`: integer setting the number of points extracted from the mesh to construct the training set at each epoch loop
- `patience`: integer setting how many epoch loops the system can go on without progressing, after that the trial is ended

An automatization of the hypertuning by hand and using Keras Tuner has already been led. Nevertheless, some work must still be done to assure a low validation error with minimal cost of time and hardware. A few bugs, impeding a proper convergence, also seems to persist in some of our implementations.

3.2 Pseudo-code

Solving PDEs using neural networks (PINN method)

Input a,b,c
Output d

a ← c
b ← a
function resursion(a,b)
    return a

3.3 Activation functions

3.4 PDE example

We want to solve the following PDE using the algorithm described on section 3.2 with some activation functions of the section 3.3.

$$\Delta\psi(x,y) + \psi(x,y) \cdot \frac{\partial\psi(x,y)}{\partial y} = f(x,y) \quad \text{on} \quad \Omega = [0,1]^2 \tag{3.1}$$

with boundary conditions $\psi(0,y) = \psi(1,y) = \psi(x,0) = 0$ and $\frac{\partial\psi}{\partial y}(x,1) = 2\sin(\pi x)$ and $f(x,y) = \sin(\pi x)(2 - \pi^2 y^2 + 2y^3\sin(\pi x))$.
This problem has a analytical solution ψ_t s.t $\psi_t(x,y) = y^2 sin(\pi x)$. Thus, to solve it and compare the results we define our loss function like $\mathcal{L} = ||\Delta\psi(x,y) + \psi(x,y) \cdot \frac{\partial\psi(x,y)}{\partial y} - f(x,y)||_2$ and the approximated solution like $\psi_a(x,y) = F(x,y)N(x,y) + A(x,y)$ with:

- $F(x,y) = \sin(x-1)\sin(y-1)\sin(x)\sin(y)$
- $A(x,y) = y\sin(\pi x)$

3.5 Jax approach

3.5.1 Jax library

Jax is a python library built using lax architecture, which makes it high performance and highly recommended for simulations that have a high computational cost. Also, because of the way it is used to implement a neural network, it is possible to parallelize several steps of the simulation so that it runs faster. Therefore, due to these characteristics, we chose to do some tests with it.

3.5.2 Solving with hyperbolic tangent

On the image below we can see the results obtained for the PDE of the section 3.4 using tanh.

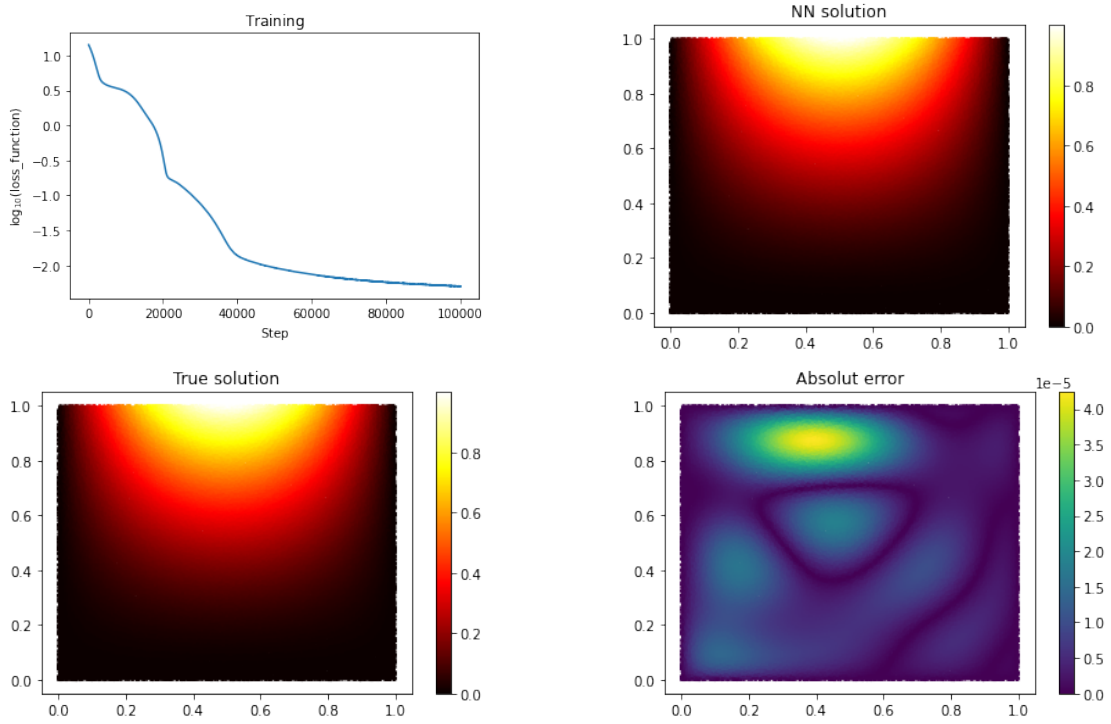


Figure 3.2: Results using Jax and hyperbolic tangent

3.5.3 Solving with sigmoid

On the image below we can see the results obtained for the PDE of the section 3.4 using sigmoid.

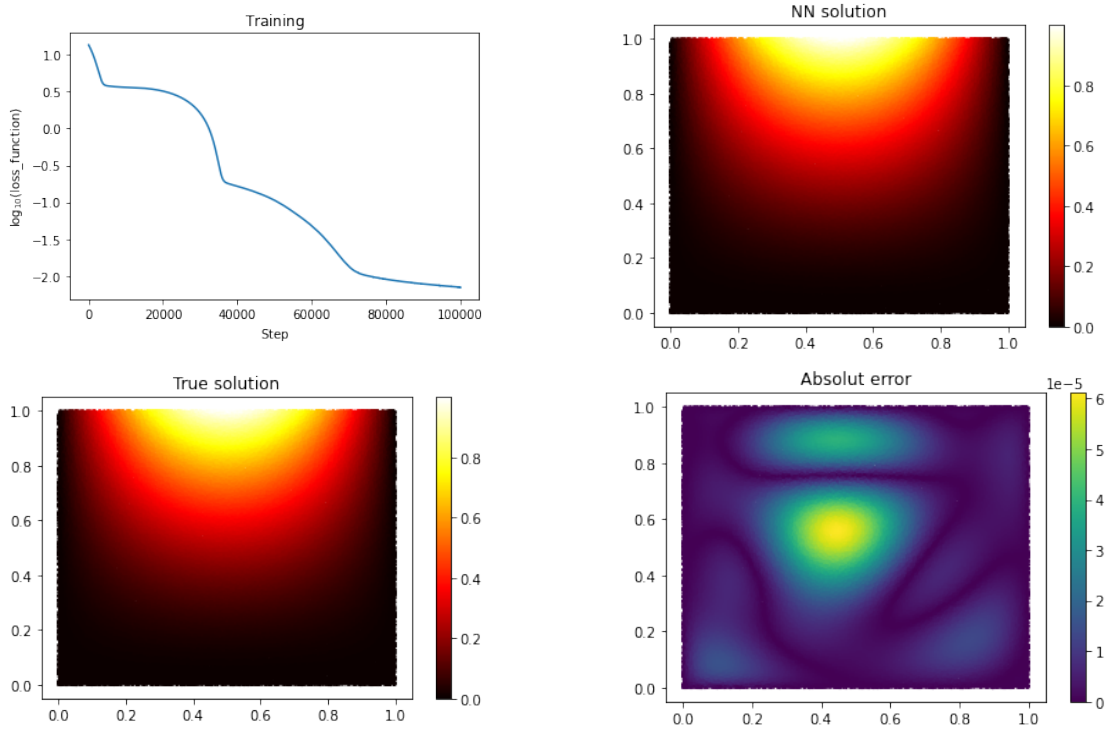


Figure 3.3: Results using Jax and sigmoid

3.5.4 Solving with elu

On the image below we can see the results obtained for the PDE of the section 3.4 using elu.

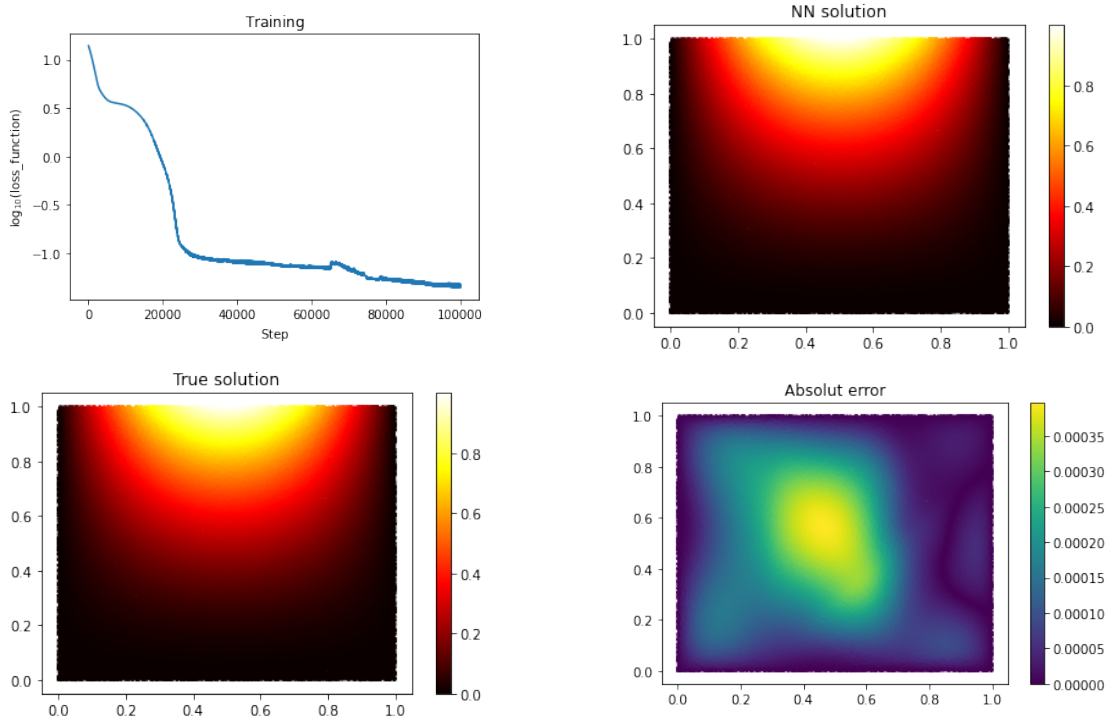


Figure 3.4: Results using Jax and elu

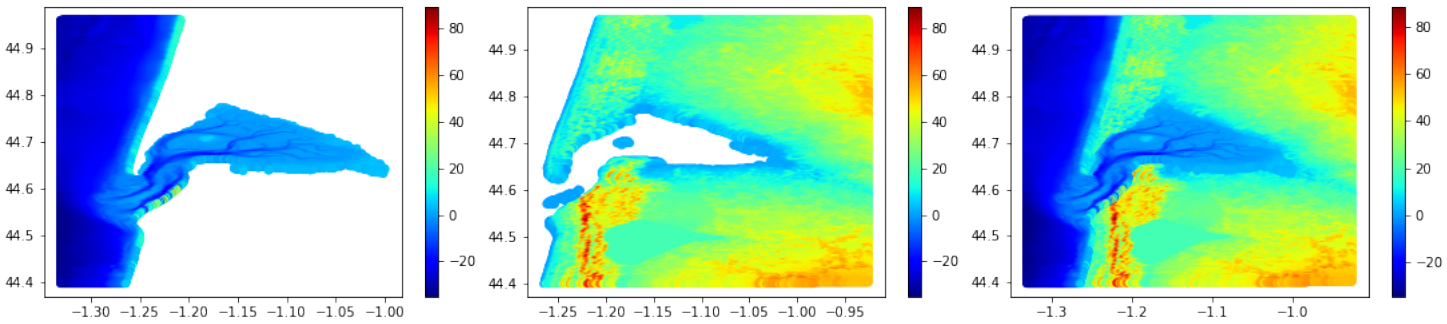
3.5.5 Analysis

According to the results obtained, the elu activation function takes longer to converge using the same parameters. Also, it is observed that the hyperbolic tangent provided a smaller absolute error for the same number of iterations.

Chapter 4 - Model

4.1 Arcachon basin

To do the simulation it is necessary to choose a location that has a lot of data available and a favorable geography, so we chose the Arcachon basin to do our simulation. The figure below shows the topology and bathymetry of this region. The dataset was obtained from Shom France and OpenTopoData.

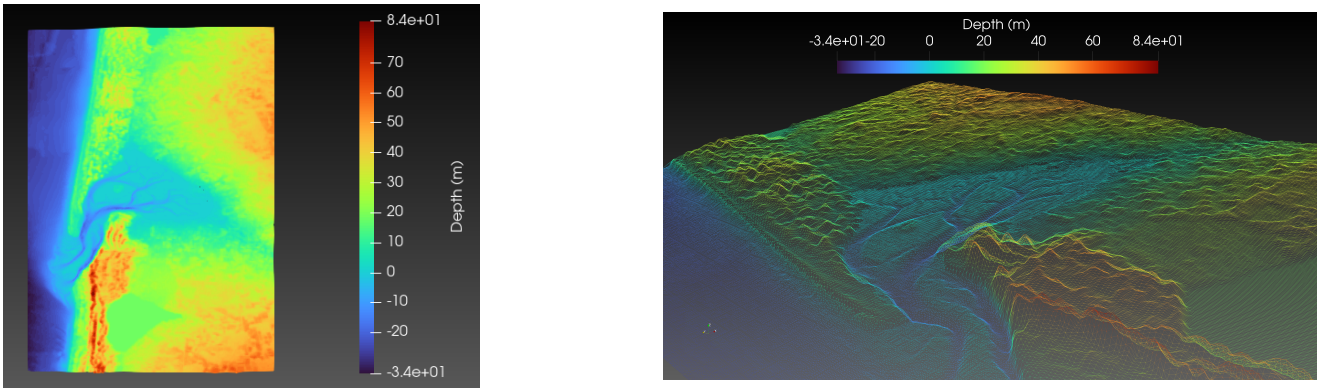


(a) Bathymetry (b) Topography (c) Topography and bathymetry

Figure 4.1: Real datas for topography and bathymetry, on scale is the depth in meters

4.2 Our approach

With the data obtained from the topology and topography of this region, the delaunay method from the PyVista library was used to make the mesh. However, due to the way the data is collected in real life, there are very sharp variations in the height of the relief. Thus, it is necessary to smooth these aspects, for this, we used the k-nearest neighbors (k-NN) with k=7 to make a mean and update the depth for each element in order to obtain a more regular structure. The figure below shows the mesh obtained for the dataset mentioned before.



(a) Topography and bathymetry (b) Wireframe

Figure 4.2: Arcachon basin mesh

4.3 Parallel processing

The obtained structure has about 280000 elements and according to the simulations performed on chapter 3, a very high number of loops will be required for the neural network to provide a good solution. However, due to the dimensions of the Mesh, the computational cost is very high, so a different approach is needed to do the simulation. A very effective way to do this is to use parallel computing, i.e. the domain is divided into several subdomains that will be processed in different cores so that the same task is divided into small subtasks to speed up the final operation. So at each step of the main loop the neural net is put to train in the sub-domains, and then at the end of each loop the performance of the net is evaluated. This procedure is described in the pseudo-code below.

Gradient descent with parallel computing

Input NN_parametres, p the number of simultaneous subtasks, loss_function
Output new parametres

repeat until convergence
  get a training set and divide it into p-subsets with the same number of elements
  for each n-processor **do**
    evaluate loss_function of the n-subset
  end for
  concatenate the p-set values obtained in the same training set order
  make gradient descent and update the parametres

- To do this in Python we can use vmap function of Jax library to vectorize the gradient descent

4.4 Mild slope equation

Chapter 5 - Simulation

Chapter 6 - Discussion of the results

Chapter 7 - Conclusion

7.1 Conclusion

7.2 Perspectives for new works and future improvements

Bibliography