Deep Learning and Dirichlet Problem.

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I wrote this note because the question of approximation functions is a question that fascinate me since I discovered the polynomial approximation of continuous functions on compact sets.

When I have some free-time, I read some articles and I found a series of articles that I studied.

1 Introduction

Recently, the work of E and Yu [5], shows that deep neural networks are numerically efficient to approwimate a solution of the Dirichlet problem.

Traditionally, when we try to approximate a function u, we do so by summing elementary functions. For example, if $u \in C(K, \mathbb{R})$ where $K \subset \mathbb{R}^d$ is a compact then we know that for any $\varepsilon > 0$ there exists a polynomial such that

$$|u - P_\epsilon|_\infty < \epsilon.$$

Here,

$$P = \sum_{\alpha \in \mathbb{N}^d} a_\alpha x^\alpha.$$

Similarly, by the Fejér's Theorem, if f is a continuous 2π periodic function, we know that it can be approximated by a trigonometric polynomial of the form

$$\sum_{j \in \mathbb{N}} a_j \cos jx + b_j \sin jx.$$

Each time sums were used.

Some mathematicians have recently wondered whether functions could be approximated by compounds instead of sums.

Where the compound is the application

$$\circ(f, g) \mapsto f \circ g.$$

Can functions that are solutions, in the strong or weak sense, of differential equations (PDEs) be approximated by composition some elementary functions?

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To do this, some mathematicians have used deep neural networks. Among the first are the works of Lee and Kang [1], as well as those of Dissanayake, M. [2], Phan-Thien, Takeuchiand Kosugi [3], Lagaris, I.E., Likas, A., and Fotiadis, [4].

For an overview, see Beck's paper [6].

2 Deep-Rietz Algorithm,[5]

The Dirichlet problem can be stated in several equivalent ways.

One of them consists in transforming the PDE problem into a functional minimisation problem, [7].

Proposition 1 ([7]; Proposition 3.1.20)**.** *Let Ω be a bounded open set of $\mathbb{R}^N$ and $f \in H^{-1}(\Omega)$. Then there exists a unique solution u to the problem:*

$$u \in H_0^1(\Omega) \quad \forall v \in H_0^1(\Omega) \quad < f, v >_{H^1(\Omega)\times H_0^1(\Omega)} = \int_\Omega \nabla u \nabla v.$$

Plus, u is the unique solution of

$$u \in H_0^1(\Omega) \quad -\Delta u = f \quad in \quad D'(\Omega)$$

and also of the minimisation problem:

$$J(u) = \min\left\{J(v) \quad v \in H_0^1(\Omega)\right\}, \tag{1}$$

Where

$$J(v) = \frac{1}{2}\int_\Omega |\nabla v|^2 - < f, v >_{H^1(\Omega)\times H_0^1(\Omega)}.$$

E and Wang have proposed an algorithm, called Deep-Riez [5], to approximate such a solution.

The minimised functional that they considered is defined by :

$$L : u \mapsto \int_\Omega \frac{1}{2}\left(|\nabla u(x)|^2 - f(x)u(x)dx\right). \tag{2}$$

The neural network defined by [5] has a finite number of blocks in which we apply two linear transformations.

We give θ the set of parameters of our network and

$$x \mapsto z_\theta(x) = f_n \circ f_{n-1} \circ ... \circ f_1(x)$$

with,

$$\forall i \quad f_i(s) := \phi(W_{i,2}\phi(W_{i,1}s + b_{i,1}) + b_{i,2}) + s.$$

Where $(W_{i,1}, W_{i,2}, b_{i,1}, b_{i,2}) \in \mathbb{R}^{m\times m} \times \mathbb{R}^m \times \mathbb{R}^m$. ϕ is an activation function, here they use the function $\phi : x \mapsto \max 0, x^3$. But there is a lot of other functions, see [8] for more details.

The authors of [5] note that the regularity of ϕ plays an important role in the convergence of the algorithm.

Then, given z_θ we find u by the equation

$$u = az_\theta + b \tag{3}$$

we will note $\Theta = \{a, b, \theta\}$ which is of finite cardinal.

The function u now depends on the parameters a, b, θ. The idea is to minimise a functional with respect to its parameters.

By sub-setting the expression of (3) in (2) we consider a finite dimensional minimisation problem:

$$\min_{\Theta} L(u_\theta). \tag{4}$$

In practice, edge conditions are difficult to encode with neural networks so we slightly modify the (2) by adding an edge term of the form

$$\lambda \int_{\partial\Omega} u_\theta^2 ds,$$

for a parameter $\lambda > 0$.

To optimize with respect to Θ they used stochastic gradient descent wich is commonly used for deep neuronal networks.

Given a sample of points $(\theta_1, ..., \theta_n)$, we want to minimize,

$$\min_{\theta} \frac{1}{N} \sum_{1 \leq k \leq N} H_k(\theta).$$

The stochastics gradient update formula is,

$$\theta^{k+1} = \theta^k - \eta \bigtriangledown H_{\gamma_k}(\theta^k) \tag{5}$$

Where η is the learning rate and γ_k are i.i.d random variables uniformly distributed over $1, ..., N$.

Dans le cas étudié par E et Wang, l'itération s'écrit, [5] :

$$\theta^{k+1} = \theta^k - \eta \frac{1}{N} \sum_{1 \leq k \leq N} \bigtriangledown_\theta G(x_{j,k}, \theta^k).$$

Where $G(x) = \frac{1}{2}\left(|\bigtriangledown u(x)|^2 - f(x)u(x)\right)$ for each k, $\{x_{j,k}\}$ is a set of points in Ω that are randomly sampled with uniform distribution.

We refer the reader to the "Numerical Results" section of [5] to see the very promising numerical results.

A few years later, [11] a first article by demonstrates from a theoretical point of view the convergence of the Deep-Riez numerical method. And establishe a lot of theoritical results such as density theorems.

Then, in [9], P.Dondl, J.Müller and M.Zeinhofer, provide convergence guarantees for the Deep Ritz Method for abstract variational energies. Their results cover nonlinear variational problems such as the p-Laplace equation or the Modica–Mortola energy with essential or natural boundary conditions. They also some uniform convergence thoerems.

We also would like to attract the attention of the reader that tere exist other deep methods. There is a paper from J.Sirignano and K.Spiliopoulos wich propose a deep Galerkin method, [10].

3 Study of the theoretical convergence guarantees for dirichle problem,[11]

Let $(\Theta)_n$ be sets of parameters of neural networks that we assume to be universal approximators in $H_0^1(\Omega)$ for $n \to \infty$. The authors introduce the following objective functions

$$L : \Theta_n \to \mathbb{R} \quad \theta \mapsto \int_\Omega \frac{1}{2} \left(|\bigtriangledown u_\theta(x)|^2 - f(x) u_\theta(x) \right) - n \int_{\partial\Omega} u_\theta^2(s) ds. \qquad (6)$$

where u_θ is the network arising from the parameters θ and $f \in L^2(\Omega)$ is a right hand side.

Theorem 1. *[[11]] Let $(\theta_n)_{n\in\mathbb{N}}$ be a sequence of quasi-minimisers of the objective functions, meaning*

$$L_n(\theta_n) \leq \inf_{\theta\in\Theta_n} L_n(\theta) + \delta_n,$$

where $\delta_n \to 0$. Then $(u_{\theta_n})_{n\in\mathbb{N}}$ converges to the solution u of the Dirichlet problem (1), both weakly in $H^1(\Omega)$ and strongly in $L^2(\Omega)$.

A remarkable fact in their proof is that, the only moment where they use the hypothesis "$\partial\Omega$ is Lipschitz, is for the proof of the lemma 7 :

Lemma 1. *[[11]] Let $\Omega \subseteq \mathbb{R}^d$ be an open and bounded set with Lipschitz boundary. Let further $r > 0$ be fixed and consider the set $M \subset H^1(\Omega)$ defined as*

$$M := \left\{ u \in H^1(\Omega) \mid \frac{1}{2} \int_\Omega |\nabla u|^2 \, dx + \int_{\partial\Omega} u^2 \, ds - f(u) \leq r \right\}. \quad (5)$$

Those functions satisfy a Poincaré type inequality of the form

$$\|u\|_{L^2(\Omega)} \leq C(\|\nabla u\|_{L^2(\Omega)} + 1), \quad (6)$$

where C only depends on r and Ω.

Proof. The proof consists of two steps. First, we will show that the inequality (5) implies that M cannot contain arbitrarily large, constant functions, and second, we prove that a failure of the Poincaré inequality (6) means that $\mathcal{M}$ contains any large, constant function; hence the assertion follows.

Step 1. Let $\xi \in \mathbb{R}$ be a constant function in M. We will show that there is some fixed $C > 0$ depending only on r, $\|f\|_{H^1(\Omega)}$, and $|\partial\Omega|$ such that $|\xi| \leq C$.

Using a scaled version of Young's inequality with $\varepsilon|\Omega|^{1/2} \leq |\partial\Omega|/2$, we compute

$$r \geq \int_{\partial\Omega} \xi^2 \, ds - f(\xi) \geq |\xi|^2|\partial\Omega| - \|f\|_{H^1(\Omega)}\|\xi\|_{H^1(\Omega)} = |\xi|^2|\partial\Omega| - \|f\|_{H^1(\Omega)}|\Omega|^{1/2}|\xi|$$

.

$$\geq \frac{|\xi|^2}{|\partial\Omega|} - C(\varepsilon)\|f\|^2_{H^1(\Omega)} - \varepsilon|\Omega| \cdot |\xi|^2$$

$$\geq \frac{1}{2|\partial\Omega|}|\xi|^2 - C(\varepsilon)\|f\|^2_{H^1(\Omega)}.$$

Thus, we can solve for $|\xi|$ and find a uniform bound in terms of r, $\|f\|_{H^1(\Omega)}$, and $|\partial\Omega|$.

Step 2. Now, we assume that the inequality fails and will show that this implies that M contains arbitrarily large constant functions. Assume, therefore, that there is a sequence $(u_k) \subset M$ such that

$$\|\nabla u_k\|_{L^2(\Omega)} + 1 \leq \frac{1}{k}\|u_k\|_{L^2(\Omega)}.$$

This inequality implies that $\|u_k\|_{L^2(\Omega)} \to \infty$, and hence, for every large but fixed $R > 0$, we may assume that $\|u_k\|^{-1}_{L^2(\Omega)}R \leq 1$ and set Let $v_k = u_k(R\|\nabla u_k\|^{-1}_{L^2(\Omega)})$. By the star shape of M, the v_k form a sequence in M, and the inequality yields, upon multiplying,

$$\|\nabla v_k\|_{L^2(\Omega)} + R\frac{\|u_k\|_{L^2(\Omega)}}{\|\nabla u_k\|_{L^2(\Omega)}} \leq R \to 0. \quad (7)$$

As $\|v_k\|_{L^2(\Omega)} = R$, and (7) implies a bound on $\|\nabla v_k\|_{L^2(\Omega)}$, we extract a weakly $H^1(\Omega)$ convergent subsequence $v_j \rightharpoonup v$ with limit v in M due to the weak closedness of M. Also, from (7) we deduce that

$$\nabla v_j \rightharpoonup \nabla v = 0 \text{ weakly in } L^2(\Omega)^n,$$

and thus, there is a constant $\xi \in \mathbb{R}$ such that $v(x) = \xi$ almost everywhere in Ω. To identify ξ, we employ the Rellich compactness theorem (see Alt, 1992), which yields that $v_j \to v$ strongly in $L^2(\Omega)$. Together with $\|v_j\|_{L^2(\Omega)} = R$, we conclude

$$R = \|v\|_{L^2(\Omega)} = |\Omega|^{1/2}|\xi|,$$

and as $R > 0$ was arbitrary, this shows that M contains any large, constant function, which manifests the desired contradiction.

Note that Rellich's theorem requires some regularity of the boundary of Ω. We assumed that it locally is the graph of a Lipschitz continuous function, but the lemma above holds whenever the embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$ is compact. $\square$

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