DEEP NITSCHE METHOD: DEEP RITZ METHOD WITH ESSENTIAL BOUNDARY CONDITIONS

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Abstract. We propose a method due to Nitsche (Deep Nitsche Method) from 1970s to deal with the essential boundary conditions encountered in the deep learning-based numerical method without significant extra computational costs. The method inherits several advantages from Deep Ritz Method [6] while successfully overcomes the difficulties in treatment of the essential boundary conditions. We illustrate the method on several representative problems posed in at most 100 dimensions with complicated boundary conditions. The numerical results clearly show that the Deep Nitsche Method is naturally nonlinear, naturally adaptive and has the potential to work on rather high dimensions.

1. Introduction

Recently there is a surge of interest in solving partial differential equations by deep learning-based numerical methods [5, 11, 6, 9, 15, 2]. However, there are few attempts to deal with the boundary conditions, particularly the essential boundary conditions, which is the main objective of the present work. These methods allow for the compositional construction of new approximation spaces from various neural networks. Such constructions are usually free of a mesh so that they are in essence meshless methods. The shape functions in the approximation spaces are in general non interpolatory, which makes the implementation of the essential boundary conditions not an easy task. Many approaches toward dealing with the essential boundary conditions have been proposed over the past fifty years; we refer to [1, §7.2] for a review.

In fact, an efficient method for imposing the essential boundary conditions has been proposed by Nitsche in the early 1970s [14]. This method was revived to deal with the elliptic interface problems and the unfitted mesh problems; we refer to [4] for a review of the progress in this direction. In the context of the meshless method, Nitsche’s idea has been proved to be an efficient approach to deal with boundary conditions in the framework of partition of unity method [8] as well as
generalized finite element method [1]. In this work, we incorporate the idea of Nitsche to deal with the essential boundary conditions in the framework of Deep Ritz Method [6]. We call this new algorithm the Deep Nitsche Method. In the next part, we introduce the energy formulation of the method, and then we present the numerical results for solving some mixed boundary value problems with regular and singular solutions in two dimensions and also for problems in high dimensions up to 100. In particular, we compare Deep Nitsche Method with Deep Ritz Method and another method based on least-squares variational formulation in all the examples. Finally we conclude with some remarks.

2. DEEP NITSCHE METHOD

We consider the mixed boundary value problem posed on $\Omega \subset \mathbb{R}^d$:

\begin{align}
\begin{cases}
-\nabla \cdot (A \nabla u) &= f, & \text{in } \Omega, \\
u &= g_D, & \text{on } \Gamma_D, \\
(A \nabla u) \cdot n &= g_N, & \text{on } \Gamma_N,
\end{cases}
\end{align}

where $A \in \mathbb{R}^{d \times d}$ is a symmetrical matrix satisfying

$$\Lambda \sum_{i=1}^{d} \xi_i^2 \leq \sum_{i,j=1}^{d} A_{ij}(x) \xi_i \xi_j \leq \lambda \sum_{i=1}^{d} \xi_i^2 \quad \text{for a.e. } x \in \Omega \text{ and } (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d.$$

The boundary $\Gamma_D \cup \Gamma_N = \partial \Omega$ and $\Gamma_D \cap \Gamma_N \neq \emptyset$.

The energy functional associated with the above boundary value problem in the sense of Nitsche [14] is

\begin{align}
I[v] := \frac{1}{2} \int_{\Omega} A \nabla v \cdot \nabla v \, dx - \int_{\Gamma_D} v A \nabla v \cdot n \, d\sigma(x) + \frac{\beta}{2} \int_{\Gamma_D} v^2 \, d\sigma(x) \\
- \int_{\Omega} f v \, dx - \int_{\Gamma_D} g_D (\beta v - A \nabla v \cdot n) \, d\sigma(x) - \int_{\Gamma_N} g_N v \, d\sigma(x),
\end{align}

where $\beta$ is a parameter to be determined later on. We minimize $I[v]$ over certain trial space $\mathcal{H}$ that will be defined later on. The resulting optimization problem is solved by the Stochastic Gradient Descent (SGD) method [7 §8].

\begin{align}
\hat{u} = \arg\min_{v \in \mathcal{H}} I[v].
\end{align}

The associated variational problem is: find $\hat{u} \in \mathcal{H}$ such that

\begin{align}
a(\hat{u}, v) = \ell(v) \quad \text{for all } v \in \mathcal{H},
\end{align}

where the bilinear form $a$ and the linear functional $\ell$ are defined by

\begin{align}
a(u, v) &= \int_{\Omega} A \nabla u \cdot \nabla v \, dx + \int_{\Gamma_D} (u (\beta v - (A \nabla v) \cdot n) - v (A \nabla u) \cdot n) \, d\sigma(x), \\
\ell(v) &= \int_{\Omega} f v \, dx + \int_{\Gamma_D} g_D (\beta v - A \nabla v \cdot n) \, d\sigma(x) + \int_{\Gamma_N} g_N v \, d\sigma(x) \quad v \in \mathcal{H},
\end{align}
respectively.

To prove the well-posedness of (2.4), we need prove the coercivity of \(a\), and the boundedness of \(a\) and \(\ell\). We make the following

**Assumption**: There exists a constant \(C_{\text{inv}}\) such that for all \(v \in \mathcal{H}\),

\[
\|\nabla v\|_{L^2(\Gamma_D)} \leq C_{\text{inv}}\|\nabla v\|_{L^2(\Omega)}.
\]

Define a norm

\[
\|v\|^2 = \|\nabla v\|^2_{L^2(\Omega)} + \|v\|^2_{L^2(\Gamma_D)}.
\]

By Friedrich’s inequality, \(\|\cdot\|\) is equivalent to the standard \(H^1\)-norm.

**Lemma 2.1.** Let **Assumption** (2.5) is valid and if \(\beta > 2\Lambda^2 C_{\text{inv}}^2 / \lambda\), then

\[
a(v, v) \geq \tilde{\lambda}\|v\|^2 \quad \text{for all} \quad v \in \mathcal{H},
\]

where \(\tilde{\lambda} = \min(\lambda - 2\Lambda^2 C_{\text{inv}}^2 / \beta, \beta / 2)\).

**Proof.** For any \(v \in \mathcal{H}\),

\[
a(v, v) \geq \lambda \int_\Omega |\nabla v|^2 \, dx + \beta \int_{\Gamma_D} v^2 \, ds(x) - 2 \int_{\Gamma_D} v(A\nabla v) \cdot n \, ds(x).
\]

Using Cauchy-Schwartz inequality and the assumption (2.5), we obtain

\[
\left| \int_{\Gamma_D} v(A\nabla v) \cdot n \, ds(x) \right| \leq \Lambda \|v\|_{L^2(\Gamma_D)} \|\nabla v\|_{L^2(\Gamma_D)}
\]

\[
\leq \frac{\beta}{4} \|v\|^2_{L^2(\Gamma_D)} + \frac{\Lambda^2}{\beta} \|\nabla v\|^2_{L^2(\Gamma_D)}
\]

\[
\leq \frac{\beta}{4} \|v\|^2_{L^2(\Gamma_D)} + \frac{\Lambda^2 C_{\text{inv}}^2}{\beta} \|\nabla v\|^2_{L^2(\Omega)}.
\]

Combining the above two equations, we obtain (2.6). \(\Box\)

The boundedness of \(a\) and \(\ell\) may be proved in a similar way. The well-posedness of the variational problem boils down to the inverse assumption (2.5), which is natural for the case when \(\mathcal{H}\) consists of polynomials, i.e.,

\[
\|\nabla v\|_{L^2(\Gamma_D)} \leq C h^{-1/2} \|\nabla v\|_{L^2(\Omega)},
\]

where \(h\) is the mesh size of the triangulation. This means that we need to take \(\beta = c_0 h^{-1}\) for certain large \(c_0\), such choice is standard in finite element literature. However, we do not know whether such inverse inequality is true for functions in \(\mathcal{H}\) that are constructed from various neural networks in compositional manner. The only exception is the function constructed from the Gaussian networks [13], which does not seem apply to the present case because it employ the distance between the centers as a measure of discretization.

The trial functions space \(\mathcal{H}\) is modeled by ResNet [10]. The component of ResNet is shown in Figure 1. The input layer is a fully connected layer with \(m\) hidden nodes,
Figure 1. The component of ResNet

which maps $x$ from $\mathbb{R}^d$ to $\mathbb{R}^m$. Assume that $\sigma$ is a scalar activation function and let $\phi$ be the tensor product of $\sigma$ as $\phi(x) = (\sigma(x_1), \cdots, \sigma(x_m)) \in \mathbb{R}^m$, then

$$s_1 = \phi(W_1 x + b_1),$$

where $W_1 \in \mathbb{R}^{m \times d}, b_1 \in \mathbb{R}^m$. The hidden layers is constructed by $l$ residual blocks. Each block contains two fully connected layers and one residual connection layer. The $i$-th block takes the form

$$s_{i+1} = \phi(W_{2,i}\phi(W_{1,i}s_i + b_{1,i}) + b_{2,i}) + s_i,$$

where $W_{1,i}, W_{2,i} \in \mathbb{R}^{m \times m}$ and $b_{1,i}, b_{2,i} \in \mathbb{R}^m$.

The output layer is a fully connected layer with one hidden node. The approximation solution may be expressed as

$$\hat{u}(x; \theta) = W_2 s_{l+1} + b_2,$$

where $W_2 \in \mathbb{R}^{1 \times m}$ and $b_2 \in \mathbb{R}$, the parameter set $\theta$ is defined as

$$\theta = \{ W_1, W_2, b_1, b_2, W_{1,i}, W_{2,i}, b_{1,i}, b_{2,i} \mid i = 1, \ldots, l \}.$$
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epochs. In each epoch, we randomly sample 128 points inside the domain Ω and

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and the energy functional associated with the Least-squares is

in finite element method. The energy functional associated with boundary value

problem (2.1) for Deep Ritz Method reads as

Noticing that one residual block contains two fully connected layers and one residual

connection, the number of trainable parameters is 1141. An Adam optimizer is

employed to train with the learning rate 0

. In all the examples, we let Ω be the unit hypercube as Ω = (0, 1)

network with five residual blocks and ten hidden nodes per fully connected layer.

Numerical Experiments

3.

3.1. Two dimensional examples. The solution u is approximated by a neural

network with five residual blocks and ten hidden nodes per fully connected layer.

Noticing that one residual block contains two fully connected layers and one residual

connection, the number of trainable parameters is 1141. An Adam optimizer is

employed to train with the learning rate 0.001[12]. We train the model for 50000

epochs. In each epoch, we randomly sample 128 points inside the domain Ω and

33 points on each edge of ∂Ω.

In the first example, we solve the Laplace equation with a smooth solution

\[ u(x, y) = \cos(\pi x)\sin(\pi y). \]

The boundary Γ_D = (0, 1) × \{0, 1\} and Γ_N = \{0, 1\} × (0, 1) and we compute f, g_D

and g_N by (2.1). We report the relative errors

\[ e_{L^2} = \frac{\|u - \hat{u}\|_{L^2}}{\|u\|_{L^2}}, \quad e_{H^1} = \frac{\|u - \hat{u}\|_{H^1}}{\|u\|_{H^1}}, \quad e_{H^2} = \frac{\|u - \hat{u}\|_{H^2}}{\|u\|_{H^2}} \]

in Table[1] for three methods with different penalized parameters β.
Table 1. The smooth solution in $d = 2$

| $\beta$ | $e_{L^2}$ | $e_{H^1}$ | $e_{H^2}$ |
|---------|-----------|-----------|-----------|
| Deep Nitsche Method | | | |
| 50 | 3.948e-2 | 6.668e-2 | 2.111e-1 |
| 500 | 6.492e-2 | 6.782e-2 | 1.585e-1 |
| 5000 | 2.029e-2 | 4.135e-2 | 1.569e-1 |
| 50000 | 1.270e-1 | 2.041e-1 | 4.592e-1 |
| Deep Ritz Method | | | |
| 50 | 2.732e-2 | 4.822e-2 | 1.136e-1 |
| 500 | 1.068e-2 | 3.069e-2 | 1.143e-1 |
| 5000 | 5.154e-2 | 1.008e-1 | 2.933e-1 |
| 50000 | 9.642e-1 | 9.663e-1 | 9.489e-1 |
| Least-Squares Method | | | |
| 50 | 5.086e-3 | 2.995e-3 | 4.570e-3 |
| 500 | 4.160e-3 | 2.564e-3 | 6.857e-3 |
| 5000 | 5.787e-3 | 9.322e-3 | 2.965e-2 |
| 50000 | 4.946e-2 | 5.909e-2 | 1.174e-1 |

It seems all three methods give comparable accuracy, and the difference between the errors with parameter $\beta$ varying from 50 to 5000 are negligible, while $\beta$ with very big value seems a bad choice. It is worthwhile to mention that $\beta = 5000$ seems the best for the Deep Nitsche method, while $\beta = 500$ seems the best for the Deep Ritz method and the least-squares method.

In the second example, we consider

\[
\begin{align*}
-\Delta u(x) &= 0, \quad x \in \Omega, \\
u(x) &= u(r, \theta) = r^{1/2} \sin(\theta/2), \quad x \in \partial \Omega,
\end{align*}
\]

where $\Omega = (-1, 1)^2 \setminus (0, 1)^2$ is an L-shaped domain. This problem admits an analytical solution $u(x) = u(r, \theta) = r^{1/2} \sin(\theta/2)$, which belongs to $H^s(\Omega)$ with $s < 3/2$. In fact, such solution usually stands for the singular part of the general situation [10]. We report the errors in Table 2. We have not computed the error in $H^2$ norm because $\|u\|_{H^2}$ is obviously unbounded. In view of Table 2, it seems that all three methods are robust with respect to the parameter $\beta$, and Deep Nitsche method seems the most accurate method for approximating the singular solution.

In the last example in two dimensions, we test problem with a nonconstant coefficient matrix $A$. The set up is the same with the previous example. Let

\[
A = \begin{pmatrix}
(x + 1)^2 + y^2 & -xy \\
-xy & (x + 1)^2
\end{pmatrix},
\]
DEEP NITSCHE METHOD

Table 2. The singular solution in $L$–domain

| $\beta$  | $e_{L^2}$   | $e_{H^1}$   |
|----------|-------------|-------------|
| Deep Nitsche Method                   |
| 50       | 7.070e-3    | 8.211e-2    |
| 500      | 7.570e-3    | 9.107e-2    |
| 5000     | 1.730e-2    | 1.885e-1    |
| 50000    | 4.959e-2    | 2.993e-1    |
| Deep Ritz Method                       |
| 50       | 1.055e-2    | 7.565e-2    |
| 500      | 9.487e-3    | 1.124e-1    |
| 5000     | 1.982e-2    | 2.011e-1    |
| 50000    | 6.542e-2    | 4.783e-1    |
| Least-Squares Method                    |
| 50       | 1.530e-2    | 1.170e-1    |
| 500      | 6.755e-3    | 1.015e-1    |
| 5000     | 2.145e-2    | 1.241e-1    |
| 50000    | 7.434e-2    | 1.951e-1    |

and

$$u(x, y) = x^3 y^2 + x \sin(2\pi xy) \sin(2\pi y),$$

where $\Gamma_D = \{1\} \times (0,1) \cup (0,1) \times \{1\}$ and $\Gamma_N = \{0\} \times (0,1) \cup (0,1) \times \{0\}$. We calculate $f$, $g_D$ and $g_N$ according to (2.1). The relative errors $e_{L^2}$, $e_{H^1}$ and $e_{H^2}$ are reported in Table 3.

In view of Table 3, it seems all methods are quite robust with respect to the penalized parameter, and the least-squares gives the best results even in case of large $\beta$.

3.2. High dimensional examples. We turn to problems in high dimensions in this part. We still employ an Adam optimizer with the learning rate 0.001 and train the model for 50000 epochs. In each epoch, we randomly sample 512 points in $\Omega$ and 16 points on each face of $\partial\Omega$.

In the first example, we consider a less smooth solution in 20 dimensions

$$u(x) = \left(\sum_{i=1}^{20} x_i^2\right)^{5/2}, \quad x \in (0,1)^{20}$$

with a pure Dirichlet boundary condition. We calculate $f$ and $g_D$ by (2.1). This example has been tested in [8] with a particle-partition of unit method. We approximate the solution by a neural network with five residual blocks and 50 hidden nodes per fully connected layer. Thus the number of trainable parameters is 26601. We report the relative errors in Table 4.
Table 3. Results for problem with coefficient in $d = 2$

| $\beta$ | $e_{L^2}$ | $e_{H^1}$ | $e_{H^2}$ |
|---------|------------|------------|------------|
| Deep Nitsche Method | | | |
| 50      | 3.940e-1  | 7.923e-1  | 1.156e0    |
| 500     | 6.121e-2  | 7.416e-2  | 2.011e-1   |
| 5000    | 2.441e-2  | 6.358e-2  | 1.768e-1   |
| 50000   | 6.902e-2  | 1.463e-1  | 3.587e-1   |
| Deep Ritz Method | | | |
| 50      | 8.901e-2  | 1.063e-1  | 2.068e-1   |
| 500     | 3.945e-2  | 6.079e-2  | 1.737e-1   |
| 5000    | 4.272e-2  | 1.106e-1  | 4.919e-1   |
| 50000   | 1.951e-1  | 3.235e-1  | 5.667e-1   |
| Least-Squares Method | | | |
| 50      | 2.593e-2  | 5.821e-2  | 7.888e-2   |
| 500     | 1.345e-2  | 3.282e-2  | 5.881e-2   |
| 5000    | 3.658e-2  | 3.564e-2  | 5.888e-2   |
| 50000   | 8.185e-2  | 5.413e-2  | 7.555e-2   |

Table 4. Less smooth solution in 20 dimensions

| $\beta$ | $e_{L^2}$ | $e_{H^1}$ | $e_{H^2}$ |
|---------|------------|------------|------------|
| Deep Nitsche Method | | | |
| 50      | 1.962e-2  | 6.887e-2  | 2.186e-1   |
| 500     | 2.517e-2  | 8.051e-2  | 5.411e-1   |
| 5000    | 1.584e-2  | 6.112e-2  | 4.659e-1   |
| 50000   | 2.098e-2  | 7.653e-2  | 3.837e-1   |
| Deep Ritz Method | | | |
| 50      | 2.102e-2  | 5.902e-2  | 3.962e-1   |
| 500     | 1.215e-2  | 4.788e-2  | 3.831e-1   |
| 5000    | 1.351e-2  | 5.612e-2  | 1.553e-1   |
| 50000   | 1.102e-2  | 4.650e-2  | 4.424e-1   |
| Least-Squares Method | | | |
| 50      | 4.486e-2  | 7.156e-2  | 1.861e-1   |
| 500     | 1.434e-2  | 5.442e-2  | 1.921e-1   |
| 5000    | 2.049e-2  | 5.484e-2  | 2.103e-1   |
| 50000   | 1.242e-2  | 4.704e-2  | 2.333e-1   |

In view of Table 3, we observe that all three methods give comparable results and all three methods are even more robust with respect to the penalized parameter $\beta$. The same conclusion is valid for the next example for higher dimensions.
In the second example, we consider a smooth solution in 100 dimensions.

\[ u(x) = \exp \left( \frac{1}{100} \sum_{i=1}^{100} x_i \right) , \quad x \in (0,1)^{100} \]

with a pure Dirichlet boundary condition. We compute \( f \) and \( g_D \) by (2.1). The exact solution \( u \) is approximated by a neural network with five residual blocks and 100 hidden nodes per fully connected layer, and the number of trainable parameters is 111201. We report the relative errors in Table 5. It shows that our method has potential to work for rather high dimensions.

### Table 5. Smooth solution in 100 dimensions

| \( \beta \)  | \( \epsilon_{L^2} \) | \( \epsilon_{H^1} \) | \( \epsilon_{H^2} \) |
|----------------|----------------|----------------|----------------|
| Deep Nitsche Method |
| 50  | 8.611e-4  | 5.014e-3  | 2.075e-2  |
| 500 | 7.795e-4  | 4.466e-3  | 1.826e-2  |
| 5000 | 3.224e-3  | 5.977e-3  | 2.098e-2  |
| 50000 | 2.291e-3  | 5.368e-3  | 2.023e-2  |
| Deep Ritz Method |
| 50  | 1.590e-3  | 4.800e-3  | 1.869e-2  |
| 500 | 7.028e-3  | 8.984e-3  | 2.355e-2  |
| 5000 | 7.992e-4  | 4.609e-3  | 2.126e-2  |
| 50000 | 2.291e-3  | 5.368e-3  | 2.023e-2  |
| Least-Squares Method |
| 50  | 5.689e-3  | 7.716e-3  | 2.374e-2  |
| 500 | 8.759e-4  | 4.845e-3  | 2.235e-2  |
| 5000 | 1.118e-3  | 3.915e-3  | 1.662e-2  |
| 50000 | 1.121e-3  | 6.444e-3  | 2.740e-2  |

Based on Nitsche’s idea and representing the trial functions by deep neural network, we propose a new method to deal with the complicated boundary conditions. The test examples show that the method has the following advantages:

(1) It deals with the mixed boundary conditions in a variational way without significant extra costs and it fits well with the stochastic gradient descent method.

(2) It works on the problems in low dimensions as well as high dimensions. It also has potential to work for problem in rather high dimensions.

(3) The method is less sensitive to the penalized parameter, by contrast to that for the traditional trial space \([8]\). This is more pronounced in high dimensions.
We also systematically compare Deep Nitsche Method with Deep Ritz Method and least-squares method for regular as well as singular solution, for low dimensional problems as well as high dimensional problems. It seems that the new method is comparable to these two methods, while it is slightly more accurate for singular solution. There are still several issues we have not addressed such as the influence of the network structures and a systematical method to improve the accuracy, which will be pursued in our future work.

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