A comprehensive study of boundary conditions when solving PDEs by DNNs

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May 12, 2020

Abstract

Recent years have witnessed growing interests in solving partial differential equations by deep neural networks, especially in the high-dimensional case. Unlike classical numerical methods, such as finite difference method and finite element method, the enforcement of boundary conditions in deep neural networks is highly nontrivial. One general strategy is to use the penalty method. In the work, we conduct a comprehensive study of four different boundary conditions, i.e., Dirichlet, Neumann, Robin, and periodic boundary conditions, using two representative methods: deep Ritz method and deep Galerkin method. It is thought that deep Galerkin method works better for smooth solutions while deep Ritz method works better for low-regularity solutions. However, by a number of examples, we observe that deep Ritz method can outperform deep Galerkin method with a clear dependence of dimensionality even for smooth solutions and deep Galerkin method can also outperform deep Ritz method for low-regularity solutions. Besides, in some cases, when the boundary condition can be implemented in an exact manner, we find that such a strategy not only provides a better approximate solution but also facilitates the training process.

Keywords: Partial differential equations; Boundary conditions; Deep Galerkin method; Deep Ritz method; Penalty method

AMS subject classifications: 65K10, 65N06, 65N22, 65N99

1 Introduction

In the past decade, deep learning has achieved great success in many subjects, like computer vision, speech recognition, and natural language processing [1][3]
due to the strong representability of deep neural networks (DNNs). Meanwhile, DNNs have also been used to solve partial differential equations (PDEs); see for example [4,12]. In classical numerical methods such as finite difference method [13] and finite element method [14], the number of degrees of freedoms (dofs) grows exponentially fast as the dimension of PDE increases. One striking advantage of DNNs over classical numerical methods is that the number of dofs only grows (at most) polynomially. Therefore, DNNs are particularly suitable for solving high-dimensional PDEs. The magic underlying this is to approximate a function using the network representation of independent variables without using mesh points. Afterwards, Monte-Carlo method is used to approximate the loss (objective) function which is defined over a high-dimensional space. Some methods are based on the PDE itself [5,11] and some other methods are based on the variational or the weak formulation [8,12,15]. In the current work, we focus on two representative methods: deep Ritz method (DRM) proposed by E and Yu [8] and deep Galerkin method (DGM) proposed by Sirignano and Spiliopoulos [11].

In classical numerical methods, boundary conditions can be exactly enforced for mesh points at the boundary. Typically boundary conditions include Dirichlet, Neumann, Robin, and periodic boundary conditions [16]. However, it is very difficult to impose exact boundary conditions for a DNN representation. Therefore, in the loss function, it is often to add a penalty term which penalizes the difference between the DNN representation on the boundary and the exact boundary condition, typically in the sense of $L^2$ norm. Only when Dirichlet boundary condition is imposed, a novel construction of two DNN representations can be used: one for the approximation of boundary condition and the other for the approximation of function over the domain [7]. The main purpose of the current work is to provide a comprehensive study of four boundary conditions using DRM and DGM. The highest derivative in the loss function in DRM is lower than that in DGM, thus it is thought that DGM works better for smooth solutions while DRM works better for low-regularity solutions. However, by a number of examples, we observe that DRM can outperform DGM with a clear dependence of dimensionality even for smooth solutions and DGM can also outperform DRM for low-regularity solutions. Besides, in some cases, when the boundary condition can be implemented in an exact manner, we find that such a strategy not only provides a better approximate solution but also facilitates the training process.

The paper is organized as follows. First, a brief introduction of DGM and DRM, systematic treatment of four different boundary conditions using the penalty method, and how to use DNNs to solve PDEs are given in Section 2. Numerous examples with different boundary conditions are compared in Section 3. Conclusions are drawn in Section 4.
2 Methodology

The usage of a DNN to solve a PDE problem consists of three parts: the loss function, the neural network structure, and the way how the loss function is optimized over the parameter space. In what follows, we first give a brief introduction of DGM and DRM. Both methods use DNNs to approximate the PDE solution, but the main difference is the choice of loss function, which is the objective function to be optimized. Afterwards, we discuss how different boundary conditions are treated using the penalty method. We then illustrate the network structure used to approximate the PDE solution. Finally, we describe the stochastic gradient descent method which is often adopted in the optimization of loss functions.

2.1 Deep Ritz method and deep Galerkin method

Consider the following boundary value problem over a bounded domain $\Omega \subset \mathbb{R}^d$

$$
\begin{aligned}
\mathcal{L}u(x) &= f(x), & \text{in } \Omega,
\Gamma u(x) &= g(x), & \text{on } \partial\Omega,
\end{aligned}
$$

where $d$ is the dimension, $f(x)$ and $g(x)$ are given functions, $\mathcal{L}$ is a differential operator with respect to $x$, and $\Gamma$ is a boundary operator which represents Dirichlet, Neumann, Robin, or periodic boundary conditions. To proceed, we assume the well-posedness of (1).

The basic idea of solving a PDE using DNNs is to seek an approximate solution represented by a DNN in a certain sense [17]. Denote the approximate solution by $u(x; \theta)$ with $\theta$ the set of neural network parameters. Both DRM and DGM use DNNs to approximate the solution, and they only differ by the corresponding loss function. Precisely, loss functions associated to DGM and DRM in terms of $u(x; \theta)$ read as

$$
\mathcal{J}_{\text{DGM}}[u(x; \theta)] = \int_{\Omega} |\mathcal{L}u(x; \theta) - f(x)|^2 \, dx,
$$

and

$$
\mathcal{J}_{\text{DRM}}[u(x; \theta)] = \int_{\Omega} (W(u(x; \theta)) - f(x)u(x; \theta)) \, dx,
$$

respectively. DGM aims to minimize the imbalance when the approximate DNN solution is substituted into $\mathcal{L}u(x) = f(x)$ of (1) in the least-square sense [11]. DRM works in a variational sense that the variation of $\mathcal{J}_{\text{DRM}}[u(x; \theta)]$ with respect to $u(x; \theta)$ yields the associated Euler-Lagrange equation $\mathcal{L}u(x) = f(x)$ [8,15].

The inclusion of boundary conditions is done by adding a penalty term

$$
\mathcal{B}[u(x; \theta)] = \int_{\partial\Omega} |\Gamma u(x; \theta) - g(x)|^2 \, ds,
$$
and respectively, the total loss functions $I[u(x;\theta)]$ for DGM and DRM are

$$I_{DGM}[u(x;\theta)] = J_{DGM}[u(x;\theta)] + \lambda B[u(x;\theta)], \quad (2)$$

and

$$I_{DRM}[u(x;\theta)] = J_{DRM}[u(x;\theta)] + \lambda B[u(x;\theta)], \quad (3)$$

where $\lambda$ is the penalty parameter.

The optimal approximation $u^*(x;\theta^*)$ is obtained by solving the following optimization problem:

$$u^*(x;\theta^*) = \arg\min_{u(x;\theta) \in \mathcal{H}(\Omega)} I[u(x;\theta)], \quad (4)$$

where $\mathcal{H}(\Omega)$ is the set of admissible functions.

### 2.2 Boundary conditions

To illustrate the penalty method for boundary conditions in DGM and DRM, we start with the following explicit example over $\Omega = (0,1)^d$ (by default)

$$-\Delta u + \pi^2 u = f(x), \quad (5)$$

The corresponding loss terms in DGM and DRM are

$$J_{DGM}[u(x;\theta)] = \int_{\Omega} | -\Delta u(x;\theta) + \pi^2 u(x;\theta) - f(x) |^2 \, dx, \quad (6)$$

and

$$J_{DRM}[u(x;\theta)] = \int_{\Omega} \frac{1}{2} \left( |\nabla u(x;\theta)|^2 + \pi^2 u(x;\theta)^2 \right) - f(x) u(x;\theta) \, dx, \quad (7)$$

respectively.

For comparison, the exact solution is set to be $u(x) = \sum_{k=1}^d \cos(\pi x_k)$ which is smooth. $f(x)$ and $g(x)$ which can be calculated explicitly will be specified later.

#### 2.2.1 Dirichlet boundary condition

Dirichlet boundary condition reads as

$$u(x) = g(x), \ x \in \partial\Omega,$$

and the corresponding penalty term is

$$B_D[u(x;\theta)] = \int_{\partial\Omega} |u(x;\theta) - g(x)|^2 \, ds. \quad (8)$$

Thus, the total loss functions of DGM and DRM for Dirichlet boundary condition are

$$I_{DGM}[u(x;\theta)] = J_{DGM}[u(x;\theta)] + \lambda B_D[u(x;\theta)], \quad (9)$$

and

$$I_{DRM}[u(x;\theta)] = J_{DRM}[u(x;\theta)] + \lambda B_D[u(x;\theta)], \quad (10)$$

respectively.
2.2.2 Neumann boundary condition

Neumann boundary condition reads as

$$\frac{\partial u}{\partial n} = g(x), \; x \in \partial \Omega,$$

where $\frac{\partial u}{\partial n} := (\frac{\partial u}{\partial x_1}, \cdots, \frac{\partial u}{\partial x_d}) \cdot n(x)$ and $n(x)$ is the unit outer normal vector along $\partial \Omega$. The corresponding penalty term is

$$B_N[u(x; \theta)] = \int_{\partial \Omega} \left| \frac{\partial u}{\partial n}(x) - g(x) \right|^2 ds$$

Thus, the total loss functions of DGM and DRM for Neumann boundary condition are

$$I_{DGM}[u(x; \theta)] = J_{DGM}[u(x; \theta)] + \lambda B_N[u(x; \theta)],$$

and

$$I_{DRM}[u(x; \theta)] = J_{DRM}[u(x; \theta)] + \lambda B_N[u(x; \theta)],$$

respectively.

2.2.3 Robin boundary condition

Robin boundary condition reads as

$$\frac{\partial u}{\partial n} + u(x) = g(x), \; x \in \partial \Omega,$$

and the corresponding penalty term is

$$B_R[u(x; \theta)] = \int_{\partial \Omega} \left| \frac{\partial u}{\partial n}(x) + u(x; \theta) - g(x) \right|^2 ds.$$}

Thus, the total loss functions of DGM and DRM for Robin boundary condition are

$$I_{DGM}[u(x; \theta)] = J_{DGM}[u(x; \theta)] + \lambda B_R[u(x; \theta)],$$

and

$$I_{DRM}[u(x; \theta)] = J_{DRM}[u(x; \theta)] + \lambda B_R[u(x; \theta)],$$

respectively.

2.2.4 Periodic boundary condition

Periodic boundary condition over the boundary of $\Omega = (-1, 1)^d$ reads as

$$\begin{cases} u(\tilde{x}_k, -1) = u(\tilde{x}_k, 1), \\
\frac{\partial u(\tilde{x}_k, -1)}{\partial x_k} = \frac{\partial u(\tilde{x}_k, 1)}{\partial x_k}, \end{cases}$$
2 METHODS

\[ \tilde{x}_k = (x_1, \cdots, x_{k-1}, x_{k+1}, \cdots, x_d) \] for \( k = 1, \cdots, d \). The exact solution is still \( u(x) = \sum_{k=1}^{d} \cos(\pi x_k) \). Note that the penalty term \( B_P[u(x; \theta)] \) in this case consists of two terms:

\[
B_{P_1}[u(x; \theta)] = \sum_{k=1}^{d} \int_{\partial \Omega} |u(\tilde{x}_k, -1) - u(\tilde{x}_k, 1)|^2 \, ds,
\]

\[
B_{P_2}[u(x; \theta)] = \sum_{k=1}^{d} \int_{\partial \Omega} |\partial u(\tilde{x}_k, -1)/\partial x_k - \partial u(\tilde{x}_k, -1)/\partial x_k|^2 \, ds.
\]

Thus, the corresponding loss functions of DGM and DRM for periodic boundary condition are

\[
I_{DGM}[u(x; \theta)] = J_{DGM}[u(x; \theta)] + \lambda_1 B_{P_1}[u(x; \theta)] + \lambda_2 B_{P_2}[u(x; \theta)],
\] (17)

and

\[
I_{DRM}[u(x; \theta)] = J_{DRM}[u(x; \theta)] + \lambda_1 B_{P_1}[u(x; \theta)] + \lambda_2 B_{P_2}[u(x; \theta)],
\] (18)

where \( \lambda_1 \) and \( \lambda_2 \) are prescribed penalty parameters.

2.3 Network structure

The deep network structure employed here is similar to ResNet [18], which is built by stacking several residual blocks. Each residual block contains one input, two weight layers, and two nonlinear transformation operations (activation functions) with a skip identity connection and one output. In details, let us consider a network with \( n \) residual blocks. For the \( i \)-th block, let \( L^{[i]}[x] \in \mathbb{R}^m \) be the input, \( W_1^{[i]}, W_2^{[i]} \in \mathbb{R}^{m \times m} \) and \( b_1^{[i]}, b_2^{[i]} \in \mathbb{R}^m \) be the weight matrices and the bias vectors, \( \sigma(\cdot) \) be the activation function, and \( L^{[i+1]}(x) \) be the output which can be specified as

\[
L^{[i+1]}(x) = \sigma(W_2^{[i]} \cdot (\sigma(W_1^{[i]} \cdot L^{[i]}(x) + b_1^{[i]})) + b_2^{[i]}) + L^{[i]}(x).
\] (19)

The initial input \( L^{[0]}(x) = W^{[0]} x + b^{[0]} \) and the final output \( L^{[n+1]}(x) = W^{[n+1]} \), \( L^{[n]}(x) + b^{[n+1]} \) with \( W^{[0]} \in \mathbb{R}^{m \times d}, b^{[0]} \in \mathbb{R}^{m \times 1} \) and \( W^{[n+1]} \in \mathbb{R}^{1 \times m}, b^{[n+1]} \in \mathbb{R} \). The schematic picture of one residual block is given in Figure 1.
Below are several commonly used activation functions

\[ \text{relu}(x) = \max(0, x), \]
\[ \text{sigmoid}(x) = \frac{1}{1 + \exp(-x)}, \]
\[ \text{swish}(x) = \frac{x}{1 + \exp(-x)}, \]
\[ \sigma(x) = (\sin x)^3. \]

Overall, the DNN approximation of PDE solution can be written as

\[ u(x; \theta) = L^{[n+1]} \circ L^{[n]} \circ \cdots \circ L^{[1]} \circ L^{[0]}(x) \quad (20) \]

where \( \theta \) is the set of full weight and bias parameters in the neural network, i.e., \( \theta = \{ W^{[0]}, b^{[0]}, \{ W_i^{[i]}, b_i^{[i]} \}_{i=1}^n, W^{[n+1]}, b^{[n+1]} \} \). The total number of parameters is \((2mn + d + 1)(m + 1)\).

2.4 Stochastic gradient descent algorithm

Using DNNs to solve PDEs is now transferred to solve the optimization problem \(4\) with the loss function \(2\) or \(3\) over the possible DNN representations \(20\). Even the original PDE is linear, the DNN representation \(20\) can be highly
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nonlinear due to the successive composition of nonlinear activation functions. On the other hand, quadrature schemes for the high-dimensional integral in (2) and (3) run into the curse of dimensionality and Monte-Carlo method can overcome this issue. The stochastic gradient descent (SGD) algorithm and its variants play a key role in deep learning training. It is a first-order optimization method which naturally incorporates the idea of Monte-Carlo sampling and thus avoids the curse of dimensionality. At each iteration, SGD updates neural parameters by evaluating the gradient of the loss function only at a batch of samples as

\[ \theta_{k+1} = \theta_k - \epsilon_k \sum_{i=1}^{N} \nabla \mathcal{I}[u(x_i; \theta_k)], \]  

(21)

where \( \theta_k \) is the parameters of neural network at the \( k \)-th iteration, \( \epsilon_k \) is the learning rate, and \( \mathcal{I}[u(x_i; \theta_k)] \) is the loss function evaluated at the \( i \)-th sampling point. \( x_i \) are randomly generated with uniform distribution over \( \Omega \) and \( \partial \Omega \). Though better sampling strategies, such as quasi-Monte Carlo sampling [19], can be used, we stick to Monte-Carlo sampling [20] in the current work for the comparison purpose.

In our work, Adam optimizer is used to accelerate the training of the deep neural network [21]. Adam algorithm estimates first-order and second-order moments of gradient to dynamically adjust the learning rate for each parameter. The main advantage is that the learning rate at each iteration has a certain range after correction, which makes the parameter update more stable. In implementation, the global learning rate \( \epsilon \) is 0.001, the exponential decay rates of moment estimation \( \rho_1, \rho_2 \) are set to be 0.9 and 0.999, and the small constant \( \delta \) used for numerical stability is set to be \( 10^{-8} \). In addition, we use the finite difference method to approximate derivatives in the loss function.

3 Numerical results

We shall use the following relative \( L_2 \) error to measure the approximation error

\[ \text{error} = \sqrt{\frac{\int_{\Omega}(u^*(x; \theta^*) - u(x))^2 dx}{\int_{\Omega}(u(x))^2 dx}}, \]

where \( u^*(x; \theta^*) \) is the DDN approximation of DGM or DRM and \( u(x) \) is the exact solution, respectively.

3.1 Training process and dimensional dependence for four boundary conditions

For four different boundary conditions, we record the training process of DGM and DRM and measure the error in terms of dimensionality. For comparison purpose, the same setup is employed for different boundary conditions, but the network structure varies as dimensionality \( d \) increases. Typically, each neural
network contains three to four residual blocks with several neural units in each layer. The activation function we used here is swish($x$).

Figure 2 - Figure 5 record the training processes of DGM and DRM in 2D, 4D, 8D, and 16D, respectively. One general trend we have observed is that DGM converges faster than DRM in the low-dimensional case; see 2D for example, while it is the opposite in the high-dimensional case; see 16D for example. In lower dimensions, both DGM and DRM converge well. However, in 16D, a significant amount of efforts have been paid in order to achieve the convergence in DGM.

For Dirichlet boundary condition, there is a novel approach which avoids the penalty term \[ 7 \]. One can first construct a simple neural network denoted by $NN(x; \theta)$ to approximate $g(x)$ on the boundary. Then, another DNN denoted by $DNN(x; \theta)$ to approximate the PDE solution in the following trail form

$$u(x; \theta) = |NN(x; \theta) - g(x)|^\alpha \cdot DNN(x; \theta) + G(x),$$

where $\alpha \in \mathbb{R}^+$ and $G(x)$ is a smooth extension of $g(x)$ over the whole domain $\Omega$. However, this two-stage strategy does not apply to other boundary conditions. In terms of the penalty term, from Figure 2 - Figure 5, a general observation is that the damping parameter decreases from Dirichlet, Neumann, Robin, and periodic boundary conditions. Since this parameter is a bit tuned to get a better approximation for a given DNN, a larger damping parameter implies a better agreement of the DNN solution and the exact solution on the boundary. On the other hand, periodic boundary condition is the most difficult case to be approximated by a DNN.
Figure 2: Training processes of DGM and DRM for four boundary conditions in 2D. Each neural network contains three residual blocks with four neural units in each layer. The mini-batch size is 2000 in the domain and 400 on the boundary for one epoch. The penalty parameter $\lambda = 100.0$ for Dirichlet, Neumann, and Robin boundary conditions and $\lambda_1 = 10.0, \lambda_2 = 5.0$ for periodic boundary condition.
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Figure 3: Training processes of DGM and DRM for four boundary conditions in 4D. Each neural network contains three residual blocks with eight neural units in each layer. The mini-batch size is 2000 in the domain, 800 on the boundary for Dirichlet, Neumann, and Robin boundary conditions, and 8000 on the boundary for periodic boundary condition. The penalty parameter $\lambda$ for Dirichlet boundary condition, $\lambda = 100.0$ for Neumann boundary condition, $\lambda = 500.0$ for Robin boundary condition, and $\lambda_1 = 1.0, \lambda_2 = 0.5$ for periodic boundary condition.
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![Graphs showing training processes of DGM and DRM for four boundary conditions in 8D.](image)

Figure 4: Training processes of DGM and DRM for four boundary conditions in 8D. Each neural network contains three residual blocks with sixteen neural units in each layer. The mini-batch size is 2000 in the domain for Dirichlet, Neumann, and Robin boundary conditions, and 4000 in the domain for periodic boundary condition, 1600 on the boundary for Dirichlet, Neumann, and Robin boundary conditions, and 16000 on the boundary for periodic boundary condition. The penalty parameter $\lambda = 100.0$ for Dirichlet boundary condition, $\lambda = 1.0$ for Neumann boundary condition, $\lambda = 10.0$ for Robin boundary condition, and $\lambda_1 = 1.0, \lambda_2 = 0.5$ for periodic boundary condition.
Figure 5: Training processes of DGM and DRM for four boundary conditions in 16D. Each neural network contains three residual blocks with thirty-two neural units in each layer. The mini-batch size is 2000 in the domain and 3200 on the boundary. The penalty parameter $\lambda = 100.0$ for Dirichlet boundary condition, $\lambda = 1.0$ for Neumann boundary condition, $\lambda = 10.0$ for Robin boundary condition, and $\lambda_1 = 10.0, \lambda_2 = 5.0$ for periodic boundary condition. 

Table 1 records relative $L_2$ errors for DGM and DRM when $d = 2, 4, 8, 16$. The number of training epochs is set to be 10000 in 2D, 20000 in 4D, 50000 in 8D, and 100000 in 16D. Other parameters of neural network are the same as those in Figure 2 - Figure 5. Generally speaking, DGM has a better approximation accuracy in low-dimensional cases; see 2D and 4D for example, which DRM outperforms in high-dimensional cases; see 8D and 16D for example. For (5), second-order derivative appears in the formulation of DGM while only first-order derivative exists in DRM. Therefore, to some extent, this is out of expectation since the exact solution here is smooth and DGM should approximate the exact better.

3.2 Dependence on network structures

Above observations hold true over a wide range of issues, such as penalty parameter, mini-batch size, activation function, neural depth, and neural width. We will show how the approximation accuracy of DGM and DRM depends on these issues by several representative results in what follows.
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Table 1: Relative $L^2$ errors for four different boundary conditions in different dimensions. The number of training epochs is 10000 in 2D, 20000 in 4D, 50000 in 8D, and 100000 in 16D. Other parameters in DNNs are specified in Figure 2 - Figure 5.

| $d$ | Dirichlet | Neumann | Robin | Periodic |
|-----|-----------|---------|-------|----------|
|     | DGM | DRM | DGM | DRM | DGM | DRM | DGM | DRM | DGM | DRM |
| 2   | 0.0071 | 0.0236 | 0.0020 | 0.0078 | 0.0006 | 0.0065 | 0.0063 | 0.0115 |
| 4   | 0.0074 | 0.0105 | 0.0128 | 0.0336 | 0.0197 | 0.0622 | 0.0449 | 0.0514 |
| 8   | 0.0226 | 0.0256 | 0.0674 | 0.0199 | 0.0561 | 0.0221 | 0.0672 | 0.0573 |
| 16  | 0.0290 | 0.0224 | 0.1747 | 0.0368 | 0.0938 | 0.0379 | 0.0525 | 0.0617 |

3.2.1 Penalty parameter

Consider Dirichlet boundary condition in 4D. Relative $L_2$ errors of DGM and DRM are recorded in Table 2 for different penalty parameters. In theory, the damping parameter $\lambda$ shall be infinity if the exact solution is found. In practice, instead, for a given DNN, $\lambda$ shall always be a finite number. It is observed from Table 2 that the larger the penalty parameter $\lambda$ is, the better the approximation is. However, if $\lambda$ is set to be too small or too large, then the penalty term can be ignored or be dominant. This results in wrong DNN solutions, i.e., a DNN approximation satisfies the PDE but not the boundary condition or satisfies the boundary condition but not the PDE. Therefore, for a given DNN, how to choose a penalty parameter which grantees optimal approximation accuracy is of particular importance and deserves further consideration.

Table 2: Relative $L^2$ errors of DGM and DRM in terms of penalty parameter $\lambda$ for Dirichlet boundary condition in 4D. The neural network contains three residual blocks with eight neural units in each layer. The activation function is $swish(x)$. The mini-batch size is 2000 in the domain and 800 on the boundary.

| $\lambda$ | DGM | DRM |
|-----------|-----|-----|
| 0.1       | 0.2186 | 0.0185 |
| 1.0       | 0.0366 | 0.0176 |
| 10.0      | 0.0127 | 0.0196 |
| 100.0     | 0.0081 | 0.0083 |

3.2.2 Mini-batch size

Consider Robin boundary condition in 4D. Relative $L_2$ errors of DGM and DRM are recorded in Table 3 for different mini-batch sizes in the domain with fixed mini-batch size on the boundary. It is seen that the approximation accuracy of both methods improves as the mini-batch size increases with possible statistical
fluctuation. Similar results are found if the mini-batch size in the domain is fixed while the mini-batch size on the boundary is adjusted.

Table 3: Relative $L^2$ errors of DGM and DRM in terms of mini-batch size in the domain. The neural network contains three residual blocks with eight neural units in each layer. The activation function is $\text{swish}(x)$. The mini-batch size is 800 on the boundary. The penalty parameter $\lambda = 100$.

| Mini-batch size | DGM   | DRM   |
|-----------------|-------|-------|
| 500             | 0.0822| 0.0230|
| 1000            | 0.1064| 0.0266|
| 2000            | 0.0197| 0.0622|
| 4000            | 0.1026| 0.0321|

3.2.3 Activation function

Consider Neumann boundary condition in 4D. Table 4 records relative $L^2$ errors of DGM and DRM in terms of several activation functions. From Table 4 it is recognized that the choice of activation function is quite important. The failure of $\text{relu}(x)$ in DGM is due to the low regularity of activation function on one hand and the higher derivative in the loss function of DGM on the other hand. This is why a better performance of DGM for smooth solutions is expected while DRM is expected to be better for low-regularity solutions. Based on results in Section 3.1, we know that the former is not always true. In Section 3.3 the latter is not true as well.

Table 4: Relative $L^2$ error in terms of activation function. The neural network contains three residual blocks with eight neural units in each layer. The mini-batch size is 2000 in the domain and 800 on the boundary. The penalty parameter $\lambda = 500$.

| Activation function | DGM   | DRM   |
|---------------------|-------|-------|
| $\text{relu}(x)$    | 0.9992| 0.0783|
| $\text{sigmoid}(x)$ | 0.0226| 0.0136|
| $\text{swish}(x)$   | 0.0176| 0.0169|
| $(\sin x)^3$        | 0.0231| 0.0110|

3.2.4 Neural depth and neural width

Consider Dirichlet boundary condition in 4D. Table 5 and Table 6 record relative $L^2$ errors of DGM and DRM in terms of neural depth $n$ and neural width $m$, respectively. It is expected that approximation errors of DGM and DRM reduce as $n$ and $m$ increase to some extent. Unlike classical numerical methods, a systematic reduction of errors cannot be observed for DNNs.
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Table 5: Relative $L^2$ error in terms of neural depth $n$. Each neural network contains varying residual blocks with eight neural units in each layer. The activation function is swish$(x)$. The mini-batch size is 2000 in the domain and 800 on the boundary. The penalty parameter $\lambda = 100$.

| Neural depth $n$ | DGM | DRM |
|------------------|-----|-----|
| 2                | 0.0114 | 0.0193 |
| 3                | 0.0074 | 0.0105 |
| 4                | 0.0108 | 0.0057 |

Table 6: Relative $L^2$ error in terms of neural width $m$. Each neural network contains three residual blocks with varying neural units in each layer. The activation function is swish$(x)$. The mini-batch size is 2000 in the domain and 800 on the boundary. The penalty parameter $\lambda = 100$.

| Neural width $m$ | DGM | DRM |
|------------------|-----|-----|
| 4                | 0.0218 | 0.1118 |
| 6                | 0.0208 | 0.1124 |
| 8                | 0.0074 | 0.0105 |
| 10               | 0.0072 | 0.0095 |

3.3 A nonlinear problem with low-regularity solution

Note that all the previous examples are linear PDEs and their solutions belong to $C^\infty(\Omega)$. Next, we study a nonlinear PDE with low-regularity solution. The nonlinear problem over the unit sphere $\Omega = \{ x \in \mathbb{R}^d : |x| < 1 \}$ reads as

\[
\begin{aligned}
-\Delta u + u^3 &= f(x), & \text{in } \Omega, \\
u(x) &= 0, & \text{on } \partial \Omega.
\end{aligned}
\]

The exact solution $u(x) = \sin \left( \frac{\pi}{2} (1 - |x|) \right) \in C^1(\Omega)$ but $u \notin C^2(\Omega)$, and $f(x) = \frac{\pi^2}{4} \sin \left( \frac{\pi}{2} (1 - |x|) \right) + \frac{\pi}{2} \cos \left( \frac{\pi}{2} (1 - |x|) \right) \left( \frac{d-1}{|x|} \right) \sin^3 \left( \frac{\pi}{2} (1 - |x|) \right) + \frac{\pi}{2} \left( 1 - \sin \left( \frac{\pi}{2} (1 - |x|) \right) \right).

Loss functions associated to DGM and DRM are

\[
\mathcal{J}_{\text{DGM}}[u(x; \theta)] = \int_{\Omega} |-\Delta u(x; \theta) + u(x; \theta)^3 - f(x)|^2 dx,
\]

\[
\mathcal{J}_{\text{DRM}}[u(x; \theta)] = \int_{\Omega} \frac{1}{2} |\nabla u(x; \theta)|^2 + \frac{1}{4} u(x; \theta)^4 - f(x)u(x; \theta) dx,
\]

and the penalty term is

\[
\mathcal{B}[u(x; \theta)] = \int_{\partial \Omega} |u(x; \theta)|^2 ds.
\]
Thus, total loss functions of DGM and DRM with penalty are

\[ I_{\text{DGM}}[u(x; \theta)] = J_{\text{DGM}}[u(x; \theta)] + \lambda B_D[u(x; \theta)], \]  

and

\[ I_{\text{DRM}}[u(x; \theta)] = J_{\text{DRM}}[u(x; \theta)] + \lambda B_D[u(x; \theta)], \]  

respectively.

### 3.3.1 Dimensional dependence

Relative \(L^2\) errors of DGM and DRM are reported in different dimensions \(d = 2, 4, 8\). Each neural network contains three residual blocks with varying neural units in each layer. The number of neural units is 8 for 2D and 4D, and 16 for 8D. The activation function is \(\text{swish}(x)\). The mini-batch size is 2000 in the domain and 400 on the boundary in 2D, 1000 in the domain and 800 on the boundary in 4D, and 1000 in the domain and 1600 on the boundary for 8D. The penalty parameter is 50.0 for 2D, 100.0 for 4D, and 400.0 for 8D. To our surprise, DGM outperforms DRM by over one order of magnitude. Note that the exact solution is only in \(C^1(\Omega)\), the second-order derivative in space appears in DGM while only first-order derivative in space is needed in DRM. Therefore, such an observation definitely deserves further investigation. Moreover, this observation holds true over a wide range of issues, such as penalty parameter, mini-batch size, activation function, neural depth, and neural width. We will show how the approximation accuracy of DGM and DRM depends on a couple of representative issues in what follows.

Table 7: Relative \(L^2\) errors of DGM and DRM in different dimensions. Each neural network contains three residual blocks with varying neural units in each layer. The number of neural units is 8 for 2D and 4D, and 16 for 8D. The activation function is \(\text{swish}(x)\). The mini-batch size is 2000 in the domain and 400 on the boundary in 2D, 1000 in the domain and 800 on the boundary in 4D, and 1000 in the domain and 1600 on the boundary for 8D. The penalty parameter is 50.0 for 2D, 100.0 for 4D, and 400.0 for 8D.

| \(d\) | DGM | DRM |
|------|-----|-----|
| 2    | 0.0003 | 0.0090 |
| 4    | 0.0055 | 0.0777 |
| 8    | 0.0292 | 0.1603 |

### 3.3.2 Penalty parameter

Table 8 records relative \(L^2\) errors of DGM and DRM in terms of penalty parameter \(\lambda\) in 2D. Again, a better approximation accuracy is achieved for larger penalty parameter \(\lambda\). However, keeping enlarging \(\lambda\) deteriorates the approximation accuracy for a fixed DNN.
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Table 8: Relative $L^2$ errors of DGM and DRM in terms of penalty parameter $\lambda$ in 2D. Each neural network contains three residual blocks with eight neural units in each layer. The activation function is $swish(x)$. The mini-batch size is 2000 in the domain and 400 on the boundary.

| $\lambda$ | DGM   | DRM   |
|-----------|-------|-------|
| 50.0      | 0.0011| 0.0517|
| 100.0     | 0.0022| 0.0161|
| 200.0     | 0.0015| 0.0076|
| 400.0     | 0.0003| 0.0090|

3.3.3 Activation function

Table 9 records relative $L^2$ errors of DGM and DRM with respect to activation function in 4D. From Table 9 we see that $relu(x)$ still has some problem due to the same reason and $swish(x)$ is the best among all tested functions.

Table 9: Relative $L^2$ errors of DGM and DRM with respect to activation function in 4D. Each neural network contains three residual blocks with eight neural units in each layer. The mini-batch size is 1000 in the domain and 800 on the boundary. The penalty parameter $\lambda$ is 100.

| Activation function | DGM   | DRM   |
|---------------------|-------|-------|
| $relu(x)$           | 0.9990| 0.1546|
| $sigmoid(x)$        | 0.0262| 0.0881|
| $swish(x)$          | 0.0055| 0.0777|
| $(\sin x)^3$        | 0.0146| 0.0907|

3.3.4 With versus without penalty

For Dirichlet boundary condition, as discussed earlier, we can actually avoid the penalty term [7] by constructing a trail function in the form of (22). Since $\Omega$ is a unit sphere, there exists a simple way to construct a trail function which automatically satisfies the exact boundary condition. Precisely, we can build the neural network solution in the form of $u(x; \theta) = (1 - |x|)DNN(x; \theta)$, where $DNN(x; \theta)$ is the DNN approximation to be trained. This will be used for both DGM and DRM without penalty term for the comparison purpose.

Figure 6 plots training processes of DGM and DRM with or without penalty and Table 10 records the corresponding relative $L_2$ errors in 4D. Each neural network contains three residual blocks with eight neural units in each layer. The mini-batch size is 1000 in the domain and 800 on the boundary. The penalty parameter $\lambda$ is 100.0. From Figure 6 without penalty, we see that both DGM and DRM converge better. Sometimes we even see that DGM and DRM without penalty converge while do not converge in the presence of penalty term.
Besides, from Table 10 we see that DGM outperforms DRM by over one order of magnitude regardless of the penalty term, and both methods perform better by over one order of magnitude if the trial function automatically satisfies the boundary condition. These together show the great importance of boundary conditions. A better treatment not only facilitates the training process but also provides better approximation accuracy for the same network setup.

![Training processes of DGM and DRM with or without penalty.](image)

**Figure 6:** Training processes of DGM and DRM with or without penalty. Each neural network contains three residual blocks with eight neural units in each layer. The mini-batch size is 1000 in the domain and 800 on the boundary. The penalty parameter $\lambda$ is 100.0. The total number of epochs is 10000.

| With or without penalty | DGM | DRM |
|-------------------------|-----|-----|
| With penalty            | 0.0055 | 0.0777 |
| Without penalty         | 0.0002 | 0.0084 |

### 4 Conclusions

In the work, we have conducted a comprehensive study of four different boundary conditions, i.e., Dirichlet, Neumann, Robin, and periodic boundary conditions, using two representative methods: DRM and DGM. It is thought that
DGM works better for smooth solutions while DRM works better for low-regularity solutions. However, by a number of examples, we have observed that DRM can outperform DGM with a clear dependence of dimensionality even for smooth solutions and DGM can also outperform DRM for low-regularity solutions. Besides, in some cases, when the boundary condition can be implemented in an exact manner, we have found that such a strategy not only provides a better approximate solution but also facilitates the training process.

There are several interesting issues which deserves further considerations. Since the penalty method works in general, the most important one is the choice of penalty parameters. For a fixed neural structure, a good choice of these parameters not only facilitates the training process but also provides a better approximation. Another issue is to understand why DGM outperforms DRM for low-regularity problems.

Acknowledgements

This work is supported in part by the grants NSFC 11971021 and National Key R&D Program of China (No. 2018YF645B0204404) (J. Chen), NSFC 11501399 (R. Du). We are grateful to Liyao Lyu for helpful discussions. All codes for producing the results in this work are available at https://github.com/wukekever/DGM-and-DRM.
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