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A Correction and Comments on "Multi-Scale Deep Neural Network (MscaleDNN) for Solving Poisson-Boltzmann Equation in Complex Domains. CiCP, 28(5):1970–2001,2020"

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Abstract. This note provides a correction of a missing weight constant in the MscaleDNN formula and some comments on the performance of the corrected algorithm.

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Key words: Multi-scale DNN, PDE solver, deep learning.

1 Correction on a missing weight constant

Our previous paper on the multi-scale deep neural network (MscaleDNN) in [2] contains an error: a constant α_i^d or its inverse is missing outside $f_i(\cdot)$ or $f_{\theta^{n_i}}(\cdot)$ in Eqs. (2.10), (2.11), (2.14) and (2.15). The following text should replace the corresponding paragraphs in [2] to correct this error.

From (2.5), we can apply a simple down-scaling to convert the high frequency region A_i to a low frequency region. Namely, we define a scaled version of $\widehat{f}_i(\mathbf{k})$ as

$$\widehat{f}_i^{(\text{scale})}(\mathbf{k}) = \widehat{f}_i(\alpha_i \mathbf{k}), \quad \alpha_i > 1, \tag{2.9}$$

and, correspondingly in the physical space

$$f_i^{(\text{scale})}(\boldsymbol{x}) = f_i\left(\frac{1}{\alpha_i}\boldsymbol{x}\right)\frac{1}{\alpha_i^d}, \tag{2.10}$$

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or

$$f_i(\boldsymbol{x}) = \alpha_i^d f_i^{(\text{scale})}(\alpha_i \boldsymbol{x}). \tag{2.11}$$

We can see the low frequency spectrum of the scaled function $\widehat{f}_i^{(\text{scale})}(\mathbf{k})$ if α_i is chosen large enough, i.e.,

$$\operatorname{supp} \widehat{f}_i^{(\text{scale})}(\mathbf{k}) \subset \left\{ \mathbf{k} \in \mathbb{R}^d, \ \frac{(i-1)K_0}{\alpha_i} \le |\mathbf{k}| \le \frac{iK_0}{\alpha_i} \right\}. \tag{2.12}$$

Using the F-Principle of common DNNs (Ref. [27] in [2]), with iK_0/α_i being small, we can train a DNN $f_{\theta^{n_i}}(\boldsymbol{x})$, with θ^{n_i} denoting the DNN parameters, to learn $f_i^{(\text{scale})}(\boldsymbol{x})$ quickly

$$f_i^{(\text{scale})}(\boldsymbol{x}) \sim f_{\theta^{n_i}}(\boldsymbol{x}), \tag{2.13}$$

which gives an approximation to $f_i(\boldsymbol{x})$ immediately

$$f_i(\boldsymbol{x}) \sim \alpha_i^d f_{\theta^{n_i}}(\alpha_i \boldsymbol{x}) \tag{2.14}$$

and to $f(\boldsymbol{x})$ as well

$$f(\boldsymbol{x}) \sim \sum_{i=1}^{M} \alpha_i^d f_{\theta^{n_i}}(\alpha_i \boldsymbol{x}). \tag{2.15}$$

3 Numerical results with the corrected MscaleDNN (2.15)

In this section, we present several numerical tests on approximation and solving PDEs to demonstrate the necessity of the missing factor α_i in front of the subnetworks $f_{\theta^{n_i}}(\cdot)$ in (2.15), which results in faster training and lower generalization errors, as shown in Fig. 1 and later sections.

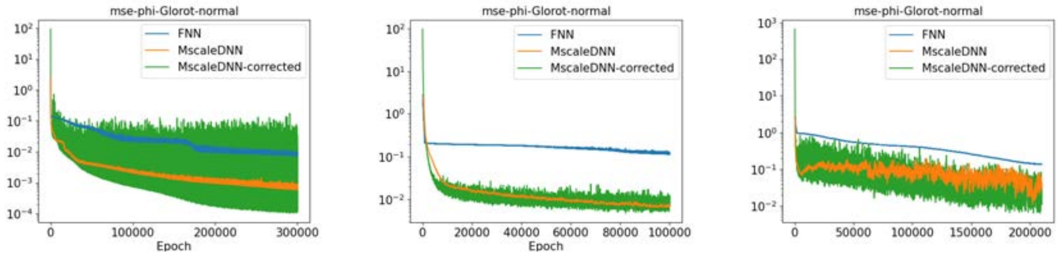
Three networks will be tested: FNN – fully connected neural network; MscaleDNN – the one missing the α_i weights; MscaleDNN-corrected – the corrected one with weight factor α_i included. In the comparison tests, we use the same compact activation functions in [2],

$$\phi(x) = \text{ReLU}(x)^2 - 3\text{ReLU}(x-1)^2 + 3\text{ReLU}(x-2)^2 - \text{ReLU}(x-3)^2. \tag{3.1}$$

3.1 Approximation of a 2-D oscillatory function

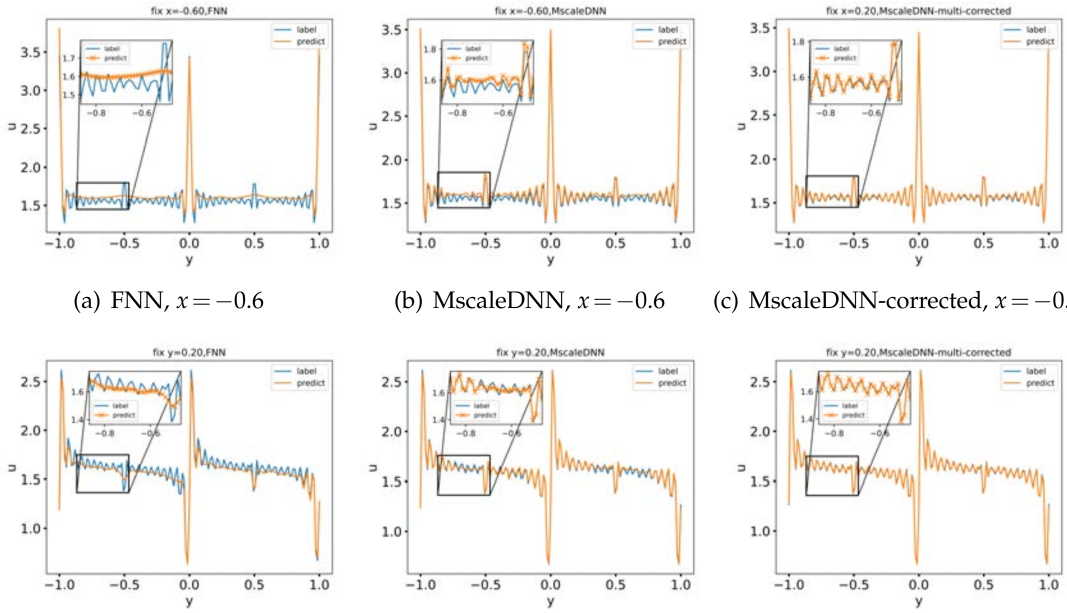
The target function for the fitting problem is $u(x,y) = \frac{1}{N^2}\sum_{m=1}^{N}\sum_{n=1}^{N} e^{\sin(2\pi m x)} e^{\cos(2\pi n y)}$, $(x,y) \in [-1,1]^2$, where $N=20$. 5000 training data at each epoch are randomly sampled from $[-1,1]^2$. DNNs are trained by the Adam optimizer with a learning rate 0.0001 and initialized with a Glorot-normal. We compare the following different network structures: (1) FNN with a size 2-1600-1600-1600-1; (2) MscaleDNN with eight subnetworks with a size 2-200-200-200-1 each and scales $\{1,2,4,8,16,32,64,128\}$; (3) MscaleDNN-corrected with eight subnetworks with a size 2-200-200-200-1 each and same scales as MscaleDNN.

In Fig. 2, we show the target function and the DNN solutions on fixed $x=-0.6$ and $y=0.2$. The MscaleDNN-corrected performs better than the MscaleDNN and FNN.



(a) Section 3.1 (b) Section 3.2 (c) Section 3.3

Figure 1: Mean squared errors of three test cases in Sections 3.1, 3.2, 3.3, respectively.



(a) FNN, $x=-0.6$ (b) MscaleDNN, $x=-0.6$ (c) MscaleDNN-corrected, $x=-0.6$

(d) FNN, $y=0.2$ (e) MscaleDNN, $y=0.2$ (f) MscaleDNN-corrected, $y=0.2$

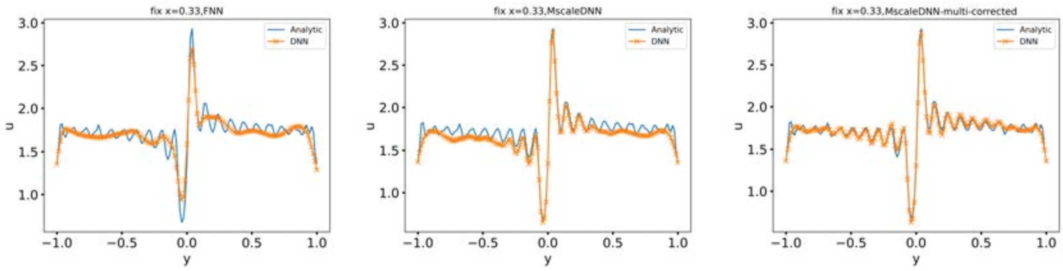
Figure 2: Different network structures in a 2-D fitting problem with $N=20$. Comparison between target function and FNN results, MscaleDNN results, and MscaleDNN-corrected results on $x=-0.6$ and $y=0.2$, respectively. The black sub-box is used for a detail view.

3.2 Solving a 2-D Poisson-Boltzmann equation with DeepRitz

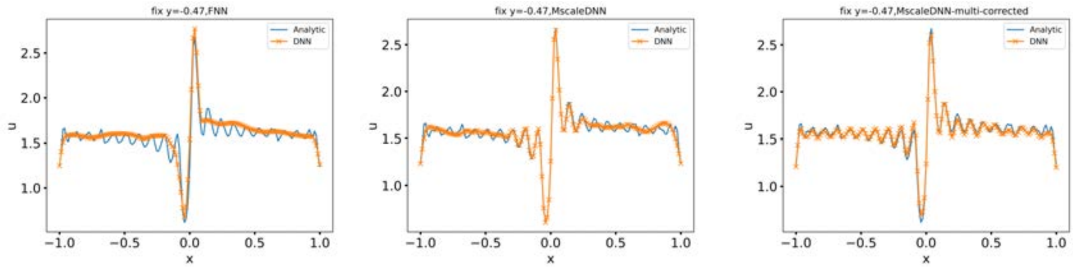
In this section, we use a variational loss, i.e., Ritz loss [1], as the training loss. We consider a 2-D Poisson-Boltzmann equation in $\Omega=[-1,1]^2$,

$$-\Delta u(x,y)+\lambda^2 u(x,y)=f(x,y), \tag{3.2}$$

where the exact solution is given by $u(x,y)=\frac{1}{N^2}\sum_{m=1}^{N}\sum_{n=1}^{N}\frac{m^2+n^2}{1+m^2+n^2}e^{\sin(2\pi mx)}e^{\sin(2\pi ny)}$.



(a) FNN, $x=0.33$ (b) MscaleDNN, $x=0.33$ (c) MscaleDNN-corrected, $x=0.33$



(d) FNN, $y=-0.47$ (e) MscaleDNN, $y=-0.47$ (f) MscaleDNN-corrected, $y=-0.47$

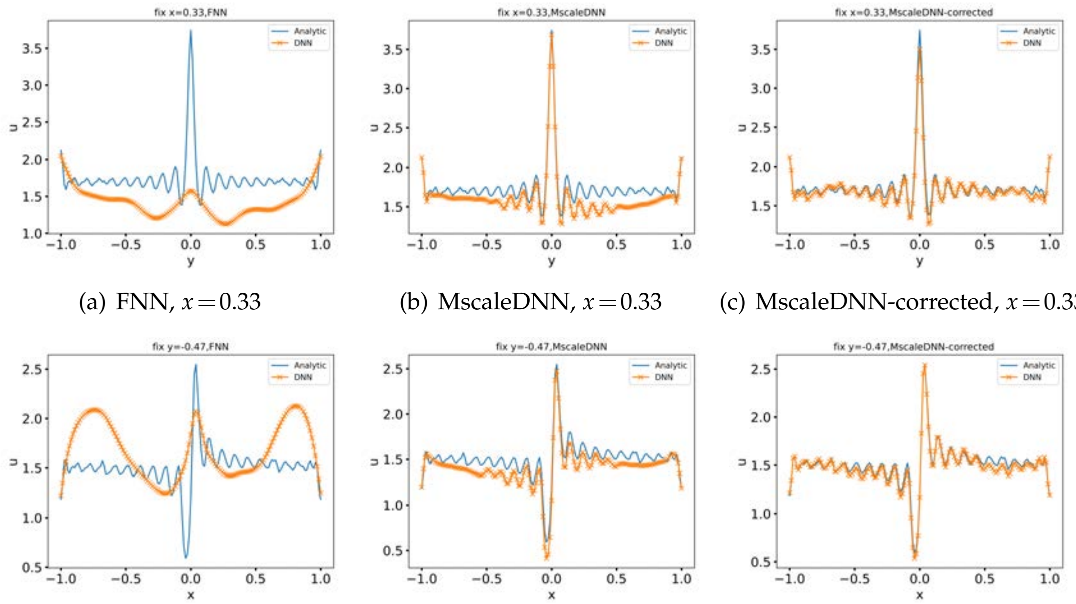
Figure 3: Different network structures in solving a 2-D Poisson-Boltzmann equation with a Ritz loss. Comparison between analytic and DNN solutions at $x=0.33$ and $y=-0.47$.

Here, we set $N=20$, $\lambda=10$. In each training epoch, we uniformly sample 5000 points inside the domain. We choose the penalty coefficient for the boundary term $\beta=5000$. DNNs are trained by the Adam optimizer with a learning rate 1e$-$5 and initialized with a Glorot-normal. We again examine the following different network structures: (1) FNN with a size 2-1600-1600-1600-1; (2) MscaleDNN with eight subnetworks with a size 2-200-200-200-1 each and scales $\{1,2,4,8,16,32,64,128\}$; (3) MscaleDNN-corrected with eight subnetworks with a size 2-200-200-200-1 each and same scales as MscaleDNN. In Fig. 3, we show the exact solution and DNN solutions on fixed $x=0.33$ and $y=-0.47$. The MscaleDNN-corrected performs better than the MscaleDNN and FNN.

3.3 Solving a 2-D Poisson equation with DeepRitz

Lastly, we use the variational loss for the training loss for a 2-D Poisson equation in $\Omega=[-1,1]^2$, i.e., $\lambda=0$ in (3.2), where the exact solution is $u(x,y)=\frac{1}{N^2}\sum_{m=1}^{N}\sum_{n=1}^{N}e^{\sin(\pi mx)}e^{\cos(\pi ny)}$.

Still we choose $N=20$. In each training epoch, we uniformly sample 5000 points inside the domain. We choose the penalty coefficient for the boundary term $\beta=1000$. DNNs are trained by the Adam optimizer with a learning rate 1e$-$5 and initialized with a Glorot-normal. We examine the following different network structures: (1) FNN with a size 2-3200-3200-3200-1; (2) MscaleDNN with eight subnetworks with a size 2-400-400-400-1



(a) FNN, $x=0.33$ (b) MscaleDNN, $x=0.33$ (c) MscaleDNN-corrected, $x=0.33$

(d) FNN, $y=-0.47$ (e) MscaleDNN, $y=-0.47$ (f) MscaleDNN-corrected, $y=-0.47$

Figure 4: Different network structures in solving a 2-D Poisson equation with a Ritz loss. Comparison between analytic solution and DNN solutions at $x=0.33$ and $y=-0.47$.

each and scales $\{1,2,4,8,16,32,64,128\}$; (3) MscaleDNN-corrected with eight subnetworks with a size 2-400-400-400-1 each and same scales as MscaleDNN.

In Fig. 4, we show the exact solution and DNN solutions on fixed $x=0.33$ and $y=-0.47$. The MscaleDNN-corrected performs better than the MscaleDNN and FNN.

4 Conclusion

The weight factors α_i^d in front of sub-networks $f_{\theta^{n_i}}(\alpha_i \boldsymbol{x})$ in (2.15) ensure better learning of higher frequency components. The weight factors are equivalent to sampling the network parameters in the outermost layer of the sub-networks in a larger range. Numerical results confirm a noticeable improvement of the performance with the corrected MscaleDNN.

References

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