Ⅰ. Introduction

Poisson Boltzmann equations play important roles in electrochemistry, solution chemistry, colloid chemistry and biophysics [2,3,4,5]. They can be used to predict electro-potentials in solvent and solute domains separated by some interface.

In this work, we introduce new methods to predict solution of Poisson Boltzmann equation (PBE) via neural network (NN). First, we generate samples via immersed finite element methods [1]. Then, neural network is trained so that the L2-difference of the IFEM-solution and NN-solution gets smaller.

The numerical solutions are reported to show proposed methods are robust to location of charges and different domain shapes.

Ⅱ. Methods

II.A. Generation of Samples

Discontinuous bubble IFEM introduced in [1] are used to generate samples. Let us describe the structure of the samples. Given a typical sample, input data has two channels. First channel is used to describe the location of interfaces. Second channel is used to describe the location of interfaces. Second channel is used to describe the location of interfaces. Second channel is used to describe the location of interfaces. Second channel is used to describe the location of interfaces.

II.B. Neural network

We employ a ResNet based neural network to predict a PB solutions [6]. Objective function is defined via the L2-difference between IFEM-solution and NN-solution of PBE. Also, Adam optimizers were used to update weights of NN.
III. Results

The evolution of the objective functions with increasing epochs-number shows that L2- differences IFEM-solutions and NN-solutions gets smaller than tolerance. We see that NN predicts the blow-ups of electro potentials near the charges. Also, the abrupt decreases of electro-potential along the interfaces are observed.

IV. Conclusion

In this work, we introduce neural network based methods to predict PBE. Numerical results show that NN-solutions converges to IFEM-solutions.

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References