The Hong Kong University of Science and Technology

Department of Mathematics

PhD THESIS EXAMINATION

Efficient Algorithms for PDE Solving and Network Pruning

By

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ABSTRACT

Efficient algorithms have become increasingly important in the field of scientific computing and machine learning due to the growing size and complexity of problems with higher dimensionality. This thesis focuses on the development of computationally efficient algorithms. Specifically, the algorithms aim to enhance computational efficiency and accuracy for these three tasks: developing neural network-based solvers for partial differential equations (PDEs), pruning deep neural networks, and solving a constrained nonconvex optimization problem in materials science. The first part of the thesis proposes the mean-field score-based transport modeling (MSBTM) algorithm, which extends the score-based transport modeling method to solve mean-field Fokker-Planck equations. This algorithm provides an efficient and accurate way to solve equations that are computationally challenging using traditional numerical methods. The algorithm's theoretical bound, on the time derivative of the Kullback-Leibler (KL) divergence between the numerical solution and the exact solution, is obtained. Moreover, an error analysis between the samples from the MSBTM algorithm and those of the associated ordinary differentiable equation is provided. Numerical experiments validate the MSBTM algorithm for different types of interacting particle systems. The second part develops an algorithm for network pruning, which reduces the number of parameters in neural networks while maintaining accuracy. The proposed pruning algorithm improves the structured sparsity in DNNs from a new perspective of evolution of features. In particular, the trajectories connecting features of adjacent hidden layers, namely feature flow, are considered. Our pruning method, feature flow regularization (FFR), penalizes the length and the total absolute curvature of the trajectories, which implicitly increases the structured sparsity of the parameters. The algorithm is shown to be effective for image classification on various datasets, including CIFAR10 and ImageNet. Finally, the last part of the thesis uses the alternating direction method of multipliers (ADMM) to solve a linearly constrained nonconvex optimization problem for grain boundary structure in materials science. The modified ADMM with an increasing penalty parameter is applied to solve the constrained minimization problem. The algorithm is shown to converge to the stationary point of the corresponding augmented Lagrangian function. In addition, sufficient conditions of quasi-convexity are identified, and the objective function is shown to be quasi-convex and to have only one minimum over the given domain. Numerical experiments demonstrate the effectiveness of the proposed algorithm, showing improvements in terms of accuracy and efficiency compared to the penalty method and the augmented Lagrangian method.

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The student's thesis is now being displayed on the reception counter in the General Administration Office (Room 3461).