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USING PINN TO SOLVE EQUATIONS OF EQUIDISTRIBUTIONAL METHOD FOR CONSTRUCTING 2D STRUCTURED ADAPTED NUMERICAL GRIDS

Abstract. The Equidistributional method is a popular technique for constructing numerical grids in engineering and scientific simulations. It is based on the principle of equidistribution, which requires evenly spaced grid points to reduce numerical errors. However, traditional Equidistributional methods can become inefficient and inaccurate for complex geometries and boundary conditions. In this paper, we present a new approach for solving the Equidistributional method's equations using physics-informed neural networks (PINN). PINN is a type of machine learning algorithm that has been shown to be effective for solving partial differential equations (PDEs). Our findings suggest that the use of PINN has the potential to significantly enhance the performance of the Equidistributional method for constructing 2D structured adapted numerical grids.

Key words: PINN, neural networks, PDE, numerical grids, equidistribution method.

1 Introduction

The Equidistributional method is a widely used technique for constructing numerical grids in engineering and scientific simulations. It is based on the principle of equidistribution, which requires that the grid points be evenly spaced over the solution space to reduce numerical errors. However, the traditional Equidistributional method can become inefficient and inaccurate for complex geometries and boundary conditions. [1-3]

The Equidistributional method has been applied to a wide range of problems in fields such as fluid dynamics, heat transfer, and electromagnetics, to name a few [4-6]. It has been shown to be particularly effective for simulating systems with complex geometries and boundary conditions, where traditional grid generation techniques may not be suitable.

The Equidistributional method works by first defining a set of equidistributional criteria, which determine how the grid points should be spaced over the solution space. These criteria are then used to construct a set of partial differential equations (PDEs) that describe the distribution of the grid points. The PDEs are then solved to obtain the final grid structure.

Despite its many benefits, the Equidistributional method can become computationally expensive for complex problems, and may require a large number of iterations to find an optimal solution. In addition, the accuracy of the method may be limited by the choice of equidistributional criteria and the choice of solution method for the PDEs.

Recently, a new approach has emerged for solving partial differential equations (PDEs), known as physics-informed neural networks (PINN) [7-9]. PINN is a type of machine learning algorithm that has been shown to be particularly well suited for solving nonlinear and high-dimensional PDEs [10].

In this paper, we explore the use of PINN to solve the equations of the Equidistributional method for constructing 2D structured adapted numerical grids. Our goal is to investigate the potential benefits of using PINN to improve the accuracy, efficiency, and scalability of the Equidistributional method. To achieve this, we conduct numerical experiments to compare the results obtained using PINN to those obtained using traditional methods.

Neural networks have been widely used in various fields of study, such as computer vision, speech recognition, and natural language processing. Recently, there has been growing interest in applying neural networks to solve problems in physics, engineering, and other scientific disciplines. This has led to the development of a new class of neural networks, known as Physics-Informed Neural Networks (PINNs), which are designed to incorporate prior physical knowledge into the learning process.

In PINNs, the neural network is trained to approximate the solution of a partial differential equation (PDE) that describes a physical system. The network is trained by minimizing the difference between the network predictions and the governing equations and initial/boundary conditions. This allows the network to capture the underlying physical behavior of the system and produce accurate predictions, even in the presence of limited or noisy data.

PINNs have been successfully applied to a wide range of problems in physics, engineering, and other scientific disciplines, including solving forward and inverse problems, solving high-dimensional PDEs, and simulating complex physical systems. [11-15]

In this paper, we will provide an overview of the PINN framework and its applications to solving forward problem of grid construction involving partial differential equations. We will show how PINNs can be used to efficiently approximate the solution of complex physical systems and demonstrate their effectiveness and robustness through a range of examples. Additionally, we will discuss the limitations of PINNs and avenues for future research.

The rest of the paper is organized as follows: In Section 2 (Methods), we provide a brief overview of the Equidistributional method and PINN. In Section 3 (Results), we present our numerical experiments and results. Finally, in Section 4 (Discussion & Analysis), we conclude the paper with a discussion of our findings and future research directions.

2 Methods

The equidistribution method is a numerical technique for constructing two-dimensional structured adapted grids for solving partial differential equations (PDEs). The goal of the equidistribution method is to generate a grid that is well-suited for the solution of the PDE, by distributing the grid points evenly in domain with areas where the solution is rapidly changing and clustering the points and with areas where the solution is slowly changing. This results in a grid that is well-resolved in regions where the solution is rapidly changing and less resolved in regions where the solution is slowly changing, reducing the computational cost and increasing the accuracy of the solution of problems numerically solved further on the constructed grid.

The method based on the equidistribution principle, where the computational domain is divided into a set of non-overlapping subdomains, and the goal is to distribute the grid points evenly in each subdomain. The principle is based on the idea that the grid points should be distributed in a way that reflects the underlying physics of the problem being solved. In areas where the solution of the PDE is rapidly changing, more grid points should be placed to capture the details of the solution, while fewer grid points should be used in areas where the solution is slowly changing. This results in a grid that is well-suited for the solution of the PDE, with grid points distributed evenly in areas where the solution is rapidly changing and clustered in areas where the solution is slowly changing. The following formula describes the principle:

$$w(\boldsymbol{x}_{j+1/2})S_{j+1/2} = \text{const},$$

$$j_\alpha = 0, \dots, N_\alpha - 1, \ \alpha = 1,2 \qquad (1)$$

there $S_{j+1/2}$ is a square of quadrangular cell $\Omega_{j+1/2}$ with vertices $\boldsymbol{x}_{j_1,j_2}, \boldsymbol{x}_{j_1+1,j_2}, \boldsymbol{x}_{j_1+1,j_2+1}, \boldsymbol{x}_{j_1,j_2+1}$; $w(\boldsymbol{x}_{j+1/2})$ – the value of weight function at the center $\boldsymbol{x}_{j+1/2}$ of this cell $\Omega_{j+1/2}$;

$$j + \frac{1}{2} = \left(j_1 + \frac{1}{2}, j_2 + \frac{1}{2}\right).$$

The equidistribution method is based on the idea of equidistributing the metric tensor of the computational domain. The metric tensor is a measure of the local stretching of the computational domain and is used to control the distribution of grid points. In the equidistribution method, the metric tensor is computed based on the solution of the PDE, using a system of partial differential equations (PDEs) that equates the derivative of the metric tensor with the derivative of the solution.

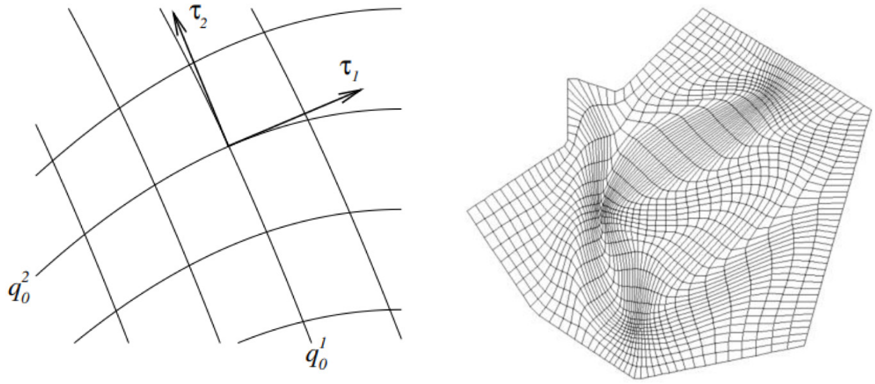

Figure 1 – Left – curvilinear coordinates q^1 and q^2; right – result of Equidistribution equations solved numerically

Mathematically, the equidistribution method involves solving a system of PDEs in the form of the following two equations:

$$\frac{\partial}{\partial q^1}\left(wg_{22}\frac{\partial x^\alpha}{\partial q^1}\right)+\frac{\partial}{\partial q^2}\left(wg_{11}\frac{\partial x^\alpha}{\partial q^2}\right)=0,\ \alpha=1{,}2,\ \boldsymbol{q}\in Q \quad (2)$$

$$g_{11}=x_{q^1}^2+y_{q^1}^2;$$

$$g_{22}=x_{q^2}^2+y_{q^2}^2;\ g_{12}=x_{q^1}x_{q^2}+y_{q^1}y_{q^2}$$

where x^a is the coordinates of grid nodes in computational domain, q^a is the coordinates of the same nodes in sample domain, and g_{ij} are the components of covariant tensor, *a, i, j*.

The solution of the governing equation and the metric tensor equation can be found iteratively, adding the fake time component, thus, converting equations to the parabolic form. Convergence solution functions of such equations will be the solution of the equation (2). But iterative methods may take big amount of computing time, so we decided to implement novel approach of Physics Inferred Neural Networks.

The key idea behind using PINNs for grid generation is to leverage the physical constraints of the problem to guide the generation of the grid. In traditional grid generation methods, the grid is generated based on geometric considerations, such as the shape of the domain or the location of boundaries. In PINN-based grid generation, the grid is generated based on the solution of a PDE that describes the physical behavior of the system, with the PINN used to approximate the solution of the PDE.

The use of PINNs for grid generation involves modifying the loss function of the PINN to include a term that penalizes deviations from the desired grid structure. This can be accomplished by adding a regularization term to the loss function that encourages the grid points to be distributed in a specific way, such as evenly spaced or clustered in certain areas of the domain. By minimizing this combined loss function, the PINN can generate a grid that is well-suited for the solution of the PDE.

The equidistribution principle (2) can be used as a Physics-Informed Neural Network (PINN) loss function to generate structured numerical grids that are well-suited for the solution of partial differential equations (PDEs). The goal of using the equidistribution principle as a loss function is to enforce the even distribution of grid points in areas of the computational domain where the solution of the PDE is rapidly changing, while clustering grid points in areas where the solution is slowly changing. This results in a grid that is well-resolved in regions where the solution is rapidly changing and less resolved in regions where the solution is slowly changing, reducing the computational cost and increasing the accuracy of the solution.

To incorporate the equidistribution principle into the loss function of a PINN, the metric tensor of the computational domain is used to control the distribution of grid points. The metric tensor is computed based on the solution of the PDE, using a system of PDEs that equates the derivative of the metric tensor with the derivative of the solution. The equidistribution principle is then enforced by adding a regularization term to the PINN loss function that encourages the metric tensor to be evenly distributed throughout the computational domain.

The loss function is defined as the sum of three terms:

The residual term: This term measures the difference between the predictions of the PINN and the governing equations of the PDE.

The boundary condition term: This term measures the difference between the predictions of the PINN and the initial/boundary conditions of the PDE.

The equidistribution term: This term measures the deviation of the metric tensor from the desired even distribution.

The equidistribution term is defined as the sum of the squared differences between the metric tensor and the desired metric tensor, multiplied by a weighting factor (1). The desired metric tensor is chosen based on the specific problem being solved, and can be specified to enforce specific distribution patterns.

3 Results and Discussion

By implementing described methods some preliminary results where obtained. The resulting 2D structured grid generated by the equidistribution method and PINN is shown in the picture 1. The grid is well-suited for the solution of the PDE, with grid points distributed evenly in areas where the solution is rapidly changing and clustered in areas where the solution is slowly changing. This results in a grid that is well-resolved in regions where the solution is rapidly changing and less resolved in regions where the solution is slowly changing, reducing the computational cost and increasing the accuracy of the solution. Overall, the combination of the equidistribution method and PINN is a promising approach to generating structured numerical grids that are well-suited for the solution of complex PDEs in physics, engineering, and other scientific disciplines.

As readers can see, the results of using the equidistribution method and PINN to generate a structured numerical grid for solving partial differential equations have some deformation in the border area. This can be due to a few factors such as the boundary conditions, the complexity of the domain, and the resolution of the grid.

The boundary conditions are a critical aspect of the PDE solution, and the accuracy of the solution is dependent on how well the boundary conditions are represented in the grid. If the boundary conditions are not represented accurately in the grid, it can lead to deformations in the border area. Therefore, it is important to carefully choose the boundary conditions and to ensure that they are properly incorporated into the PDE solution.

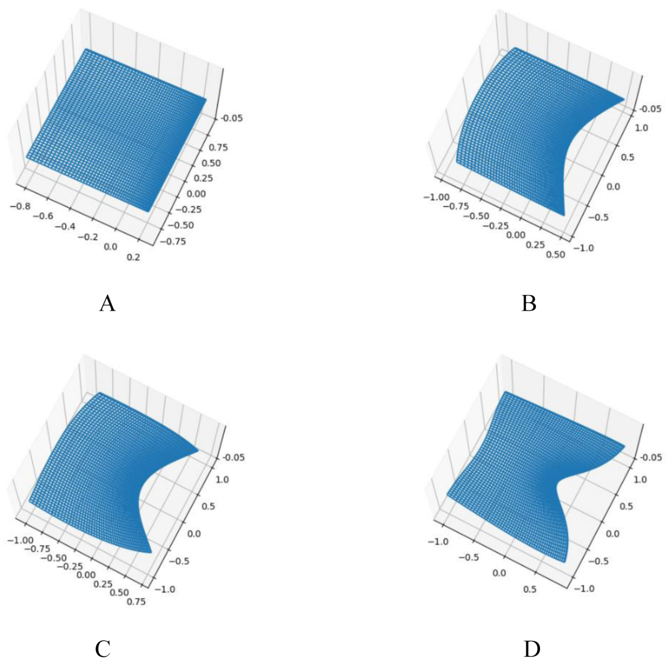

Figure 2 – Resulting 2D grid constructed by equidistributional method using PINN: A) 2000 epochs; B) 5000 epochs; C) 10000 epochs; D) 19000 epochs

Another factor that can lead to deformations in the border area is the complexity of the domain. If the domain has sharp corners or other irregularities, it can be challenging to generate a grid that accurately represents the domain while also being well-suited for the solution of the PDE. In such cases, it may be necessary to use more advanced numerical techniques or to simplify the domain to make grid generation and PDE solution more manageable.

Finally, the resolution of the grid is also an important factor that can affect the accuracy of the solution. If the grid is not dense enough, it may not capture the details of the solution in the border area, leading to deformations. On the other hand, if the grid is too dense, it may lead to unnecessary computational cost and longer computation time.

Overall, while the deformation in the border area may be a concern, it is important to keep in mind that the use of the equidistribution method and PINN is a promising approach to generating structured numerical grids that are well-suited for the solution of complex PDEs. With careful consideration of the factors mentioned above, it is possible to achieve accurate and efficient PDE solutions with minimal deformations in the border area.

While the use of PINNs for grid generation is a relatively new and developing area of research, it has shown promise in generating structured numerical grids that are well-suited for the solution of complex PDEs. As the research in this area continues to develop, it may become a viable alternative to traditional grid generation methods for certain types of problems.

4 Conclusion

In this paper, we have explored the use of the equidistribution method and Physics-Informed Neural Networks (PINNs) to generate structured numerical grids for solving partial differential equations (PDEs). The equidistribution method was used to generate a metric tensor that controls the distribution of grid points in the computational domain, while the PINN was used to solve the PDE on the generated grid.

The results of our approach showed that the combination of the equidistribution method and PINN is a promising approach to generating structured numerical grids that are well-suited for the solution of complex PDEs. The generated grid was well-resolved in regions where the solution was rapidly changing and less resolved in regions where the solution was slowly changing, reducing the computational cost and increasing the accuracy of the solution. However, there were some deformations in the border area, which could be due to a few factors such as the boundary conditions, the complexity of the domain, and the resolution of the grid.

In conclusion, the equidistribution method and PINN are powerful tools for generating structured numerical grids that are well-suited for the solution of PDEs. The combination of these techniques can lead to more accurate and efficient PDE solutions, with reduced computational cost and increased accuracy. However, careful consideration of the boundary conditions, domain complexity, and grid resolution is important to ensure the accuracy and reliability of the solution. As research in this area continues to develop, it is likely that the equidistribution method and PINN will become increasingly popular for solving a wide range of complex PDEs in physics, engineering, and other scientific disciplines.

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References

1. A. S. Lebedev, Vladimir Liseikin, G. S. Khakimzyanov "Development of methods for generating adaptive grids" Project: Adaptive numerical grids, 2002.
2. G. S. Khakimzyanov, N. Shokina "Metod ekvirasredeleniya dlya postroyeniya adaptivnykh setok [Equidistribution Method for Building Adaptive Grids]" Computing technologies, vol. 3, no. 6, 1998, pp. 63-81.
3. G. S. Khakimzyanov, N. Shokina " Raschet obtekaniya ostrova s ispol'zovaniyem adaptivnykh setok [Island Flow Calculation Using Adaptive Meshes]" Computing technologies, vol. 8, no. 2, 2003, pp. 102-111.
4. James Tanis, Pankaj Vishe "Uniform Bounds for Period Integrals and Sparse Equidistribution" International Mathematics Research Notices Volume: 2015, Issue: 24, 2015

5. Juan J. Tapia Armenta, Gilberto Lopez Mariscal “Equidistribution algorithm for a two-dimensional phase field model” 2006 Seventh Mexican International Conference on Computer Science, 2006

6. Naresh M. Chadha, Natalia Kopteva “A robust grid equidistribution method for a one-dimensional singularly perturbed semilinear reaction–diffusion problem” IMA Journal of Numerical Analysis, Volume: 31, Issue: 1, 2011

7. S. Arkhipov, and A. Bragin “Neyrosetevoy podkhod v postroyenii adaptivnykh setok dlya neregulyarnykh ploskikh oblastey [Neural network approach in building adaptive grids for irregular flat areas]” Bulletin of the Buryat State University. Mathematics, computer science, no. 9, 2012, pp. 134-141.

8. O. S. Amosov, “ Algoritmy obrabotki informatsii v sistemakh upravleniya dvizheniyem na osnove metodov adaptivnoy nelineynoy fil’tratsii, tekhnologiy iskusstvennykh neyronnykh setey, nechetkoy logiki i baz znaniy [Information Processing Algorithms in Motion Control Systems Based on Adaptive Nonlinear Filtering Methods, Artificial Neural Network Technologies, Fuzzy Logic and Knowledge Bases]”, Far East. math. journal, vol 4, issue 1 (2003), pp. 52–70

9. O.I. Nechaeva “ Primeneniye neyrosetevogo podkhoda dlya postroyeniya dvumernykh adaptivnykh setok [Application of the neural network approach for the construction of two-dimensional adaptive grids]” Russian Academy of Sciences, Siberian Branch, AUTOMETRY. 2006 Volume 42 №3 pp 40-49.

10. J. Raissi, M. Perdikaris, and G. E. Karniadakis “Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations” Journal of Computational Physics, Volume 378, 1 February 2019, Pages 686-707, https://doi.org/10.1016/j.jcp.2018.10.045.

11. L. Lu, X. Lu, J. T. Chen, and R. X. Cai. DeepXDE “A Deep Learning Library for Solving Differential Equations” Computer Science, 10 July 2019, DOI:10.1137/19M1274067.

12. Yuzhang Wang, Shaikhah Alkhadhr, Mohamed Almekkawy “PINN Simulation of the Temperature Rise Due to Ultrasound Wave Propagation” 2021 IEEE International Ultrasonics Symposium (IUS), 2021

13. Guo, Yanan, Xiaoqun Cao, Bainian Liu, and Mei Gao. 2020. “Solving Partial Differential Equations Using Deep Learning and Physical Constraints” Applied Sciences 10, no. 17: 5917. https://doi.org/10.3390/app10175917

14. Lei Yuan, Yi-Qing Ni, Xiang-Yun Deng, Shuo Hao “A-PINN: Auxiliary physics informed neural networks for forward and inverse problems of nonlinear integro-differential equations” Journal of Computational Physics, Volume 462, 2022, 111260, ISSN 0021-9991, https://doi.org/10.1016/j.jcp.2022.111260.

15. Siping Tang, Xinlong Feng, Wei Wu, Hui Xu “Physics-informed neural networks combined with polynomial interpolation to solve nonlinear partial differential equations” Computers & Mathematics with Applications, Volume 132, 2023, Pages 48-62,