Numerical Study of Dynamical System Using deep learning Approach

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Abstract: This article is devoted to developing a deep learning method to the numerical solution of the partial differential equations (PDEs). Graph kernel neural networks (GKNN) approach to embedding graphs into a computationally numerical format has been used. In particular, for investigation mathematical models of the dynamical system of cancer cells invasion in inhomogeneous areas of human tissues has been considered. Neural operators were initially proposed to model the differential operator of PDEs. The GKNN mapping features between input data to the PDEs and their solutions has been constructed. The boundary integral method in combination Green's functions for a large number of boundary conditions are used. The tools applied in this development are based on the Fourier neural operators (FNOs), graph theory, theory elasticity, and singular integral equations.

Keywords: Deep learning, Graph Kernel Network, Green's tensor.

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1. Introduction

DEEP learning is a sub-discipline of artificial intelligence that uses machine learning algorithms based on the artificial neural networks to create patterns and make predictions from large data sets [1]. We propose to solve PDEs by approximating the solution with a deep neural network (DNN) which is trained to satisfy the differential operator, initial condition, and boundary conditions [2]

The increasing adoption of deep learning across healthcare domains together with the availability of highly characterized cancer datasets has accelerated research into the utility of deep learning in the analysis of the complex biology of cancer. In this work the dynamical system of tumor cells driving in the human tissues are investigated. With the introduction of the deep learning framework, there have been numerous attempts to create more efficient approaches of numerical solutions of PDEs by using a graph kernel algorithm and a spectral decomposition of Laplacian graph approach [6]. A cancel cell network of distribution into tissues can be represented as a dynamic graph. In this paper we present a graph neural operator-based method to define mathematical problems to model the dynamical model of diffusion of tumor cells.

Cancer invasion and the ability of malignant tumor cells for directed migration and metastasis have remained a focus of research for many years. Numerous studies have confirmed the existence of two main patterns of cancer cell invasion: collective cell migration and individual cell migration, by which tumor cells overcome barriers of the extracellular matrix and spread into surrounding tissues. Each pattern of cell migration displays specific morphological features and the biochemical/molecular genetic mechanisms underlying cell migration [1]. Cancer can also spread from where it first started to other parts of the body. This process is called metastasis [2]. Cancer cells can metastasize when they break away from the tumor and travel to a new location in the body through the blood or lymphatic system. Where cancer can spread and staging. Most cancers have a tendency to spread to certain areas of the body. This has helped doctors develop staging systems that are used to classify cancers based on information about where the cancer is in the body and if it has spread from where it started [1].

Immunotherapies have revolutionized treatments for several types of cancers, but have been met with clinical trial failures in others. To improve immunotherapeutic approaches requires understanding how the immune system interacts around and within a tumor, allowing us to establish effective immunotherapeutic protocols. Mathematical modelling can help identify the mechanisms at the heart of immunotherapeutic efficacy and design successful therapeutic regimens.

2. Notations and Definitive Consepts

The mechanics of cancer cells can be described using linear elasticity theory for biomechanical systems [5]. In contrast to the molecular dynamics simulations, finite element analysis requires less computation power and can be used to model larger portions or the entire length of cancer. Therefore, finite element analysis is a useful tool to approximate and estimate the mechanical properties diffuse interface models have gained a growing interest in cancer research for their ability to investigate the mechanic-biological features during tumor progression and to provide simulation tools for personalized anti-cancer strategies at an affordable computational cost. Here we propose a diffuse interface model for tumors evolution which accounts for an interfacial structure mimicking a finite elastic confinement at the tumor boundary, possibly due either to a localized elastic stress induced by host tissue

displacements area. This model consists of the system of a partial differential equation of thermos- elasticity.
In contrast to the molecular dynamics simulations, finite element analysis requires less computation power and can be used to model larger portions or the entire length of microcells. Therefore, finite element analysis is a useful tool to approximate and estimate the mechanical properties of the microtubules. Fourier neural operators (FNOs) are used to create a neural operator pseudo oscillation system of PDEs. The relaxation dynamics of the cancer cells are described by the following system of partial differential equations:

$$\begin{array}{ll} \forall x \in D^{+} & L(\partial x,\tau)U(x,\tau) = F(x) \\ \forall z \in \partial D & [\mathrm{U}]^{+} = 0 \end{array} \quad (1)$$

where $U = (u, u_3)$, where $u = (u_1, u_2)$ is a displacement vector, u_3 is a temperature variation, $x = (x_j);\ y = (y_j); j = 1,2$-points of E^2 − two-dimensional Euclidean space,
($D^{+} \subset E^2, D^{(0)} = E^2 \backslash D^{+} \cup \partial D$) bounded by the close surface $S \in L_{(2)}(\alpha),\ \alpha > 0$ of Holder class with outward positive normal vector.
$L(\partial x,\tau) = |L_{jk}(\partial x,\tau)|_{3x3}$ is neural operator for PDEs of $L(\partial x, \partial t)$- elliptic operator of PDEs of biomechanical system described as a follow:

$$L(\partial x,\tau) = \begin{Vmatrix} (\lambda+2\mu)\Delta - \varsigma\tau^2 & -\gamma_\tau \Delta \\ -\eta\tau & \Delta - \dfrac{\tau}{\wp_\tau} \end{Vmatrix} \quad (2)$$

Where

$\varsigma > 0,\ \mu > 0, 3\lambda + 2\mu > 0,\ \wp > 0,\ \dfrac{\gamma}{\eta} > 0$ are the constants of elasticity, temperature and diffusion parameters in D^{+} domain $\gamma_\tau = \gamma_\tau(1+\tau_1\tau), \frac{1}{\mathfrak{R}_\tau} = \frac{1}{\mathfrak{R}_\tau}(1+\tau_0\tau)$
$\tau_1 \geq \tau_0 > 0$ constants of relaxation, Δ is a two-dimensional Laplacian operator; $\tau = \sigma + iq, \sigma > 0$ (corresponds to the general dynamical problems) [5],[6], $\mathrm{F} = (F_1, F_2, F_3) \subset C^{0,\alpha}(D^{+}),\ \alpha > 0$ is a given vectors.

3. Deep Learning of Green's Function

For numerically study we propose a graph neural network for the solution of the problem(1) .
There are a variety of ways to go about embedding graphs, each with a different level of granularity. In our investigations Graph Kernel Network **(GKN)** techniques on processing the entire graph have been used.
In particularly the Green's functions Artificial Neural Network (ANN) approach are used and therefor the solutions are described as follows:

$$\mathrm{U}(\mathrm{x},\tau) = -\frac{1}{2}\int_{D^{+}} G(x,y;\tau,\boldsymbol{D}^{+})F(y)\,dy \quad (3)$$

Where G(x,y) is the 2d-dimensional Green's tensor $\|G(x,y)\|_{3x3}$ [3] that represents the impulse response of the underlying system subject to homogeneous Dirichlet boundary condition, namely, for any fixed x ∈ D [5].

4. Neural Green's Function

Constructing the analytic Green's function for a given domain is in general a difficult matter, but accordingly theory of elasticity the (1) problem has regular solutions and Green's function can be represented in quadrature [4].
In order (2) neural Green's function is derived as a follow:

$$G(x,y;\tau,\boldsymbol{D}^{+}) = \sum_{j=1}^{\infty} \omega_j \varphi_j(x)\varphi_j(y) \quad (4)$$

Where $\left(\omega_{j,}\varphi_j(x)\right)$is accountable sequence of Eigen pairs.

As a result of (2) and (3) when utilizing the Green's function to obtain the solution, the exact solution and its numerical approximationˆ can be represented through

$$\mathrm{U}(\mathrm{x},\tau) = -\frac{1}{2}\sum_{J=1}^{\infty} \omega_j \left(\int_{D^{+}} \varphi_j(y)F(y)\,dy\right)\varphi_j(x) \quad (5)$$

$$U^N(\mathrm{x},\tau) = -\frac{1}{2}\sum_{J=1}^{N} \omega_j \left(\int_{D^{+}} \varphi_j(y)F(y)\,dy\right)\varphi_j(x) \quad (6)$$

In order to assumptions of Green's tensor [5] and applying the Cauchy-Schwarz inequality [4], we have

$$\mathrm{U}(\mathrm{x},\tau) = \lim_{\mathrm{N}\to\infty} \mathrm{U}^N(\mathrm{x},\tau) \quad (7)$$

Let us consider particular case of boundary conditions for (1) in finite space$(0 \leq |x| \leq 1)$, with respect to $\varphi_j(x)$ we have: $\varphi_j(0) = \varphi_j(1) = 0$
Let us introduce the following notation:

$$G(x,y) = \hat{G}(x,y,\boldsymbol{r}(x,y)), \forall x \in \boldsymbol{D}^{+}, \forall y \in \boldsymbol{D}^{+} \cup \partial\boldsymbol{D}, \quad \boldsymbol{r} = |\boldsymbol{x}-\boldsymbol{y}|$$

In order to investigate the spectral bias in the training dynamics related to (2) expand the approximation error during the training process in terms of the orthonormal eigenfunctions in the following form[7,11]:

$$\hat{G}(x,y;\tau,\boldsymbol{D}^{+}) - G(x,y;\tau,\boldsymbol{D}^{+}) = \sum_{j=1}^{\infty} \theta_j \varphi_j(x)\varphi_j(y) \quad (8)$$

Where

$$\theta_j = \int_0^1 \int_0^1 \left(\hat{G}(x,y) - G(x,y)\right) \varphi_j(x)\varphi_j(y)\,dy\,dx$$

in $(0,1)$

Here we only focus on the interior approximation error, as the Dirichlet boundary condition can be enforced by defining the L^2 loss over high frequencies $j \geq \eta$ for our neural approximation as:

$$L_k = \sum_{j=k}^{\infty} \theta_j^2 \quad (9)$$

Let us consider numerical experiments to show effectiveness of our approach in solving the one-dimensional indefinite boundary value problems, throughout the training process, we employ a fully-connected neural network with a tanh activation function [12], 14].

As a result, the approximate solution $\widehat{U}$ of problem (1) can be immediately obtained using our neural Green's function (Figure 1,2). The numerical solution using our neural Green's function has the approximation error (Figure 3).

Let us consider the particular case of boundary conditions with respect to (1).

Problem. It is required to find in D the regular solution $U = (u, u_3)^T = \|u_k\|_{3x1}$, of system (1), which satisfies the boundary condition; the displacement vector and temperature variations are given on the $x_2 = 0$ line:

$$u(x_1,0) = \psi^{(1)}(x_1),\ u_3(x_1,0) = \psi_3(x_1).$$

Therefor the solutions are described as follows:

$$u_1 = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\partial}{\partial n(y)} H\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x-y|\right)\psi_1(y)dy - \frac{1}{\pi}\iint_{x_2>0} G_1(x,z)F_1(z)dz$$

$$u_2 = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\partial}{\partial n(y)} H\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x-y|\right)\psi_2(y)dy - \frac{1}{\pi}\iint_{x_2>0} G_2(x,z)F_2(z)dz$$

$$u_3 = \frac{1}{\pi}\int_{-\infty}^{+\infty} \frac{\partial}{\partial n(y)} H\left(i\tau\sqrt{\frac{\tau}{\gamma_\tau \wp_\tau}}|x-y|\right)\psi_3(y)dy - \frac{1}{\pi}\iint_{x_2>0} G_3(x,z)F_3(z)dz$$

Where

$$G_1(x,z) = H_0^{(1)}\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x-z|\right) + H_0^{(1)}\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x^*-z|\right)$$

$$G_2(x,z) = H_0^{(1)}\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x-z|\right) - H_0^{(1)}\left(i\tau\sqrt{\frac{(\varsigma+\eta)}{(\lambda+2\mu)}}|x^*-z|\right)$$

$$G_3(x,z) = H_0^{(1)}\left(i\tau\sqrt{\frac{\tau}{\gamma_\tau \wp_\tau}}|x-y|\right) + H_0^{(1)}\left(i\tau\sqrt{\frac{\tau}{\gamma_\tau \wp_\tau}}|x^*-z|\right)$$

Where $x = (x_1, x_2)$, $x^* = (x_1, -x_2)$, $H_0^{(1)}(\ )$-is Hankel Function of the First Kind (the zero order)[5]-13].

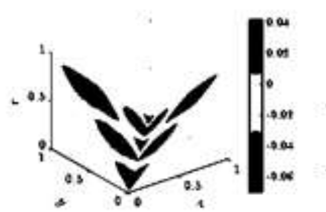

Figure 1. The numerical solution $\hat{G}(x,y)$ on the surface together for solving (1)

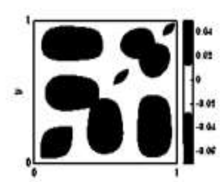

Figure 2. The numerical solution $\hat{G}(x,y)$ on the surface together with the projection into space $G(x,y)$

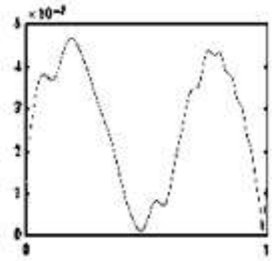

Figure3. The exact solution U and numerical solution $\widehat{U}$ using neural Green's function with the approximation error: $|U - \widehat{U}|$

5. Conclusion

In this work a novel framework for solving regular PDEs using Deep Neural Networks is developed, extended, and analyzed. A novel data-enrichment algorithm into neural Green's function framework is presented, Benefits of graph embedding in treatment being able to represent data using graph embedding offers great benefits, including:

- The embeddings can be used in machine learning prediction tasks.
- Graph embedding allows researchers to explore hidden patterns of censored cells within large networks of data.
- This greatly enhances the accuracy and efficiency of machine learning algorithms
- By identifying hidden patterns, researchers can make informed decisions and come up with better solutions for complex problems.

The method to modify the boundary problem through a deep learning algorithm to perform the long-time simulation for the rogue wave by the superior numerical errors is developed. The proposed method gives rise to the better numerical results with MI in comparison with the ones obtained by traditional methods.

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