An Alternative Method for Characterization and Comparison of Plant Root Shapes

A thesis submitted to the
College of Graduate and Postdoctoral Studies
in partial pulfillment of the requirements
for the degree of Master of Science
in the Department of School of Environment and Sustainability
University of Saskatchewan
Saskatoon

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Contents

Existed Morphological Descriptors for Root Systems

1.1 Background

...

1.1.1 Importance of Roots

...

1.1.2 Importance of Research

...

1.2 Summary of Existed Descriptors

...

1.2.1 Metric

...

1.2.2 Non-Metric

...

1.3 Problem Statements

...

1.3.1 Limitation of Data

...

1.3.2 Incompleteness and Low Efficiency

...

1.3.3 Incorrectness

...

An Alternatively Mathematical Method for Shape Description

2.1 Kac's Idea: Can One Hear the Shape of a Drum?

...

2.1.1 Interpretation

...

2.1.2 Summarize Kac's Idea

...

2.2 Extended Works of Kac's Idea: Heat Content

...

2.2.1 Mathematical Formula

...

2.2.2 Exploration of Geometrical Information

...

2.2.3 Limitations in Application

...

2.3 Numerical Methods for Solving Parabolic Partial Differential Equations

The heat equation is a critical time-dependent parabolic partial differential equation characterizing how a quantity diffuses through a given region over time. From the physical interpretation of the heat equation, its solution describes the heat distribution or temperature varying in time and positions and can be obtained uniquely by considering specific initial and boundary conditions. As described in the section 2.2, this thesis aims to calculate the asymptotic expansion of the heat content, defined as the integration of the solution over the space-dimension, for the shape description of a bounded domain. The general solution of the heat equation is in one of the two standard forms [16]. One is constituted of a series of error functions or related integrals, which is most suitable for evaluating short-time diffusion behaviour numerically. Another is in the form of a trigonometrical series, which converges rapidly for a long time. If the heat equation is defined in a cylinder, a series of Bessel functions will replace the trigonometrical series.

However, the traditional analytical techniques for solving the heat equation has many restrictions, and its applications to practical problems will exhibit difficulties. Firstly, the numerical evaluation of the analytical solutions is usually by no means trivial because they are in the form of infinite series. Secondly, either irregular geometries or discontinuities lead to the complexities, so the explicit algebraic solutions are close to non-existed. Thirdly, the purely analytical techniques can apply strictly only to the linear form of the boundary conditions and to constant diffusion properties [16].

Therefore, numerical methods and computer simulations are more helpful and applicable to find solutions to the partial differential equations (PDEs) than calculating pure analytical solutions. The techniques for solving initial-boundary value problems (IBVPs) based on numerical approximations have existed for a long time and been developed considerably including the finite-difference method (FDM), finite element method (FEM), finite volume method (FVM), boundary element method (BEM), and so forth.

2.3.1 Finite Difference Method

FDM is frequently utilized to converting the heat equation into a system of algebraically solvable equations [33]. The basic idea is to replace the derivatives in the equation by the difference quotients. For example, the FTCS (Forward Time Centered Space) scheme [59] discretizes the Laplace operator in space and the time derivative, and then implements the boundary conditions on the staggered grid for representing the original continuous problem.

Let $u(x, y, t)$ be the heat distribution at position (x, y) and time t in a $2-$dimensional homogeneous and isotropic domain Ω. It is well-known that without any internal heat sources in the domain, $u(x, y)$ satisfies the heat equation

$$u_t = D(u_{xx} + u_{yy}) \tag{2.1}$$

Note, D is a constant diffusion coefficient and u_t inidicates partial derivative with respect to time t, while u_{xx} and u_{yy} indicate second partial derivative with respect to x and y repectively.

Before the implementation of FTCS, let descrtize Ω along the $x-$axis and $y-$axis as a regular lattice. In other words, both the range of x and that of y are divided into equal intervals $\triangle l$. Also, the time is devided into equal interval δ. Let the corrdinates of a representative grid point (x, y, t) be $(i\triangle l, j\triangle l, n\delta)$, where $\triangle l$ is the distance between two neighboring sites of the lattice and δ is the time step. For simplicity, we denote the value of u at the point $(i\triangle l, j\triangle l)$ at time $n\delta$ by $u(i, j, n)$.

The difference formula for time derivative is

$$u_t = \frac{u(i,j,n+1) - u(i,j,n)}{\delta} + \mathcal{O}(\delta) \tag{2.2}$$

The difference formula for the spatial derivaive of x and y are

$$u_{xx} = \frac{u(i-1,j,n) - 2u(i,j,n) + u(i+1,j,n)}{(\triangle l)^2} + \mathcal{O}((\triangle l)^2) \tag{2.3}$$

$$u_{yy} = \frac{u(i,j-1,n) - 2u(i,j,n) + u(i,j+1,n)}{(\triangle l)^2} + \mathcal{O}((\triangle l)^2) \tag{2.4}$$

Dropping the error terms $\mathcal{O}(\delta)$ and $\mathcal{O}((\triangle l)^2)$ and substituting the Eq. 2.2, Eq. 2.3, and Eq. 2.4 into original heat equation Eq. 2.1, there will have

$$\frac{u(i,j,n+1) - u(i,j,n)}{\delta} = D(\frac{u(i-1,j,n) - 2u(i,j,n) + u(i+1,j,n)}{(\triangle l)^2} + \frac{u(i,j-1,n) - 2u(i,j,n) + u(i,j+1,n)}{(\triangle l)^2}) \tag{2.5}$$

Rearranged Eq. 2.5 as

$$u(i,j,n+1) = \frac{D\delta}{(\triangle l)^2}(u(i-1,j,n) - 2u(i,j,n) + u(i+1,j,n) + u(i,j-1,n) - 2u(i,j,n) + u(i,j+1,n)) + u(i,j,n) \tag{2.6}$$

Finally, the value of $u(i,j,n+1)$ can be expressed explicitly in terms of $u(i-1,j,n)$, $u(i+1,j,n)$, $u(i,j-1,n)$, $u(i,j+1,n)$, and $u(i,j,n)$ by

$$u(i,j,n+1) = \beta(u(i-1,j,n) + u(i+1,j,n) + u(i,j-1,n) + u(i,j+1,n)) \tag{2.7}$$

$$+ (1-4\beta)u(i,j,n) \tag{2.8}$$

$$\beta = \frac{D\delta}{(\triangle l)^2} \tag{2.9}$$

The FTCS is conditionally stable [59] because the explicit formula in Eq. 2.7 is stable if and only if $\beta \leq \frac{1}{2}$, which means

$$\delta \leq \frac{(\triangle l)^2}{2D} \tag{2.10}$$

Eq. 2.10 implies that if the spatial resolution $\triangle l$ becomes doubled, the time-step δ should be reduced by a factor of four to maintain the numerical stability, which causes the extremely tiny time-step in the high-resolution calculations. Moreover, there are three kinds of errors needed to be considered when using FDM. First of all, in the derivation of the finite-difference equations, the higher-order terms in the Taylor series are neglected, constituting the truncation error. If the time and space interval tends to 0, the truncation errors will approach 0, or the FDM is incompatible or inconsistent with the original heat equation [16]. Another class of error appearing in FDM, called round-off error, results from the loss of precision due to the computer rounding of decimal quantities. [37]. The last type of error is the discretization error, which can be reduced by decreasing the time size, grid size, or both [16]. Moreover, DFM becomes less accurate and hard to implement when the problem is defined in the irregular geometries since the heat equation must be transformed before applying the Taylor series.

2.3.2 Finite Element Method

Unlike the FDM, the finite element method (FEM) [76] divides the complicated geometries, irregular shapes, and boundaries into the union of smaller and simpler subdomains (eg. lattice, triangle, curvilinear polygons, etc.), which are called finite elements [54]. The smaller size of the finite element mesh, the more accurate the approximate solution. Therefore, FEM has great flexibilites or adaptivities [61]. For example, FEM can provide higher fidelity or higher accuracy in a local region and keep elsewhere the same. Each subdomain is locally represented by the element equation, continuous piecewise shape functions, which are finally assembled into a larger system of algebraic equations for modelling the entire problem. FEM aims to approximate the numerical solution by minimizing the associated error function to meet certain specification of the accuracy, which can be done by the parallelization. Nevertheless, FEM heavily relies on the numerical integration, where the quadrature rules sometimes cause difficulties. FEM requires an amount of human involvement in the process of building the FE model, checking the result, detecting and updating the model design. Moreover, compared with FDM, FEM demands a longer execution time and a larger amount of input data.

2.3.3 Other Numerical Techniques

Another method closely related to the FEM is the finite volume method (FVM). It converts the original heat equation into the integral forms [27]. However, the accuracy of FVM is related to the integration with respect to the time and space. Unlike the domain-type methods (e.g. FDM, FEM, FVM, etc.), the boundary element method (BEM) transforms the heat equation, defined in a given domain, into an integral equation over the boundary of the domain using the boundary integral equation method [5]. Especially, when the domain extends to infinity or the boundary is complex, BEM is more efficient in computation than other methods because of the smaller surface or volume ratio [47] since it only discretizes the boundary and fits the boundary values into the integral equation [4]. However, the matrics resulted in BEM are generally unsymmetric and fully populated, which are difficult to be solved [57].

2.3.4 Limitations in Practice

In this thesis, the heat equation defined in 2-dimensional domain, which is bounded by the border of the image and the whole root system, with millions of pixels, the extremely complex roots and various boundary conditions. Before the calculation of the heat content contained in the domain, the numerical computational techniques can be used to approximate the solutions of the heat equation, but some practical difficulities have to be considered since all the described numerical methods have an intrinsically similar feature - mesh discretization in the time and space dimension. For instance, the far more efforts are required in sovling heat equation by FDM and FVM because of the complicated boundary of the roots and non-continuous issues. Although the whole 2-dimensional root image can be regarded as a discretized domain, it is still time-consuming and challenging to trace and identify the boundary of roots, label the nodes, and generate the coordinates and connectivities among the nodes in the preprocessing stage of FEM. The finer discrtization, the more accurate approximation of the original IBVP in the numerical methods. More importantly, the heat content defined as the integration of the numerical solution of the heat equation over the space dimension should also be approximated numerically, which results in the extra effort and errors.

2.4 Monte Carlo Simulation for Approximating Heat Content

In the section 2.3, several generally utilized numerical methods [33][76] [27] [5] for solving the heat equation, and their limitations in practice are presented. In this section, one of the non-deterministic algorithms, Monte Carlo method (MCM) [63] [50], and its application in approximating the solution of the PDEs are proposed. As the weaknesses and challenges of applying the numerical techniques in solving $2-$dimensional heat equation defined in the real root images with millions of pixels and extremely complex root systems, the alternative fixed-time step Monte Carlo simulations, lattice random walks (LRWs), is designed. The most outstanding advantage of the proposed random walk model is that the integration, named the heat content, can be approximated directly based upon the probabilistic interpretation of Brownian motion and the heat equation. Finally, the methods to analyze the output of the Monte Carlo simulations and solve the sampling-related problems in the simulations are brought up theoretically.

2.4.1 Background

...

2.4.1.1 Brownian Motion

...

2.4.1.2 Probabilistic Interpretation

...

2.4.1.2.1 Survival Probability ...

2.4.1.2.2 Mean First-Passage Time ...

2.4.1.3 Random-Walk Theory

...

2.4.1.4 Monte Carlo Methods for Solving Heat Equation

...

2.4.2 Monte Carlo Simulation of Particle Diffusion: Lattice Random Walks

...

2.4.2.1 LRWs and Heat Equation

...

2.4.2.2 Algorithm of LRWs

...

2.4.2.3 Sample Size Determination

...

2.4.3 Output Analysis

...

2.4.3.1 Kaplan-Meier Estimator

...

2.4.3.2 Confidence Interval

...

2.4.3.3 Relationship Between t and τ

...

2.4.3.4 Two-Sample Statistical Tests

...

Method Validation in Annulus

3.1 Analytical Results

...

3.2 Numerical Approximation

...

3.3 Lattice Random Walks in Annulus

...

3.4 Comparesion of Numerical and Analytical Results

...

Lattice Random Walks on Artificial Images

4.1 Shape Design

...

4.1.1 Simple Shapes

...

4.1.1.1 Shape Description

...

4.1.1.2 Purpose

...

4.1.2 Complicated Shapes

....

4.1.2.1 Shape Description

...

4.1.2.2 Purpose

...

4.2 Assumption Verification

...

4.2.1 Circle and Rectangular

...

4.2.2 Artifical Branching Structures

...

4.2.3 Conclusion

...

4.3 Conclusion

...

Efficient Random Walks in Real Root Images

5.1 Description of Efficient Random Walks

...

5.2 Image Description

...

5.3 Output Analysis

...

5.3.1 Distance Matrices

...

5.3.2 Statistical Tests for Distance Matrices

...

Conclusion

6.1 Conclusion

...

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