C2: An Alternative Mathematical Method for Shape Description

I. Kac's Idea: Can One Hear the Shape of a Drum? [11]

A. Interpretations of Kac's Problem

i. When the drum vibrates, one can hear the sound, which is composed of tones of various frequencies. How much can shape features be inferred from hearing a discrete spectrum of pure tones produced by a drum?

ii. If a complete sequence of eigenvalues of the Dirichlet problem for the Laplacian can be obtained precisely, will people determine the shape of a planar?

B. Problem Statement by Mathematical Language

i. Consider a simply connected membrane Ω in the Euclidean space bounded by a smooth convex curve $\partial\Omega$ (i.e. a drum without any holes);

ii. Find a function ϕ on the closure of Ω, which vanishes at the boundary $\partial\Omega$, and a number λ satisfying $-\Delta\phi = \lambda\phi$ in Ω.

a. Δ is the Laplace operator. i.e. $\Delta = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$ in Cartesian coordinate system.

b. If there exists a solution $\phi \neq 0$, the corresponding λ is defined as a Dirichlet eigenvalue.

c. For each domain Ω, there has a sequence of eigenvalues $\lambda_1, \lambda_2, \lambda_3, ...$ corresponding to a set of eigenfunction $\phi_1, \phi_2, \phi_3, ...$

d. ϕ_k form an orthonormal basis of $L^2(\Omega)$ of real valued eigenfunctions; the corresponding discrete Dirichlet eigenvalues are positive ($\lambda_k \in \mathbb{R}^+$).

iii. An important function [8]: $h(t) = \sum_{k=1}^{k=\infty} e^{-\lambda_k t}$

a. It is a Dirichlet series.

b. It is called the heat trace or the spectral function.

c. It is smooth and converges for every $t > 0$.

C. Understanding the Problem in the Physical Context by Diffusion Theory

i. Diffusion Equation: It describes the density fluctuations of the diffusing material.

ii. $C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0})$

a. It indicates the concentration of matter (i.e. microscopic particles) at $\boldsymbol{s}$ at time t starting from $\boldsymbol{s_0}$.

b. It satisfies the diffusion equation [3]

$$\frac{\partial C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0})}{\partial t} = D\Delta C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0}) \tag{1}$$

where D is the diffusion equation. Let D be 1.

c. Initial condition: $C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0}) = \delta(\boldsymbol{s} - \boldsymbol{s_0})$ as $t \to 0$ (Dirac delta function): $\delta \neq 0$ if and only if $\boldsymbol{s} = \boldsymbol{s_0}$.

d. Boundary condition: $C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0}) = 0$ for $\boldsymbol{s} \in \partial\Omega$

e. It can be expressed in terms of eigenvalues λ_k and the corresponding normalized eigenvalues ϕ_k by: $C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0}) = \sum_{k=1}^{\infty} \phi_k(\boldsymbol{s})\phi_k(\boldsymbol{s_0})e^{-\lambda_k t}$.

iii. As $t \to 0^+$,

$$\begin{aligned}\int_\Omega C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0})d\boldsymbol{s_0} &= \int_\Omega C_\Omega(\boldsymbol{s_0}, t|\boldsymbol{s_0})d\boldsymbol{s_0} \\ &= \int_\Omega \Big(\sum_{k=1}^{\infty} \phi_k^2(\boldsymbol{s_0})e^{-\lambda_k t}\Big)d\boldsymbol{s_0} \\ &= \sum_{k=1}^{k=\infty} e^{-\lambda_k t} \\ &= h(t)\end{aligned} \tag{2}$$

where $\int_\Omega \phi_k^2(\boldsymbol{s_0})d\boldsymbol{s_0} = 1$ because of the normalization of ϕ.

D. Summarize the Results of Kac's Idea

i. As $t \to 0^+$, the leading terms of the asymptotic expansion of $h(t)$ imply the geometrical attributes of Ω

a. the total area

b. the perimeter

c. the curvature

ii. If the domain Ω has the polygonal boundary, the third term shows in the information about the interior angles of the polygon [8].

E. Conclusion

i. Strengthness

a. Proposed a noval mathematical method for the shape description without using measuring tools, i.e. rulers.

b. Other mathematicans extended Kac's idea in exploring the geomrtrical information of more complex domain with various boundary conditions [12][6][7] [17][15].

ii. Limitations

a. Except in very few cases (i.e. rectangular, disk, certain triangles), the complete sequence of eigenvalues λ_k can not be calculated [8].

b. Only the first few terms in the asymptotic expansion of $h(t)$ are explicitly available.

II. Extended Work of Kac's Idea [4][16]: Heat Content $Q_\Omega(t)$

A. Fouier's Heat Equation [2]

i. Connection with the diffusion equation Eq. 1 mentioned in Kac's paper

a. When the diffusion coefficient of the diffusion equation is independent of the density (i.e. constant diffusion coefficient), the diffusion equation is also named the heat equation.

ii. Mathematical Expression

$$\frac{\partial u(\boldsymbol{s},t)}{\partial t} = \Delta u(\boldsymbol{s},t) \tag{3}$$

iii. Mathematical interpretation

a. A deterministic model used to describe the evolution of quantities over the space and time.

B. $u(\boldsymbol{s},t)$

i. $u(\boldsymbol{s},t)$ is the general solution to the heat equation Eq. 3 providing the value of the tempretature at $\boldsymbol{s} \in \Omega$ at time t.

ii. $u(\boldsymbol{s},t) = \int_\Omega C_\Omega(\boldsymbol{s},t|\boldsymbol{s_0})\delta(\boldsymbol{s}-\boldsymbol{s_0})d\boldsymbol{s_0}$

a. Consider $C_\Omega(\boldsymbol{s},t|\boldsymbol{s_0})$ as the distribution of the heat at $\boldsymbol{s}$ after time t when initially there is only one single hot spot at $\boldsymbol{s_0}$.

b. $C_\Omega(\boldsymbol{s},t|\boldsymbol{s_0})$ is the foundamental solution to the Eq. 3.

c. $C_\Omega(\boldsymbol{s},t|\boldsymbol{s_0})$ is called the heat kernel of Ω.

d. $u(\boldsymbol{s},t)$ is the convolution of the initial condition with the heat kernel of the domain.

C. Heat Content: $Q_\Omega(t)$

i. $Q_\Omega(t) = \int_\Omega u(\boldsymbol{s},t)d\boldsymbol{s}$

ii. As $t \to 0^+$, $Q_\Omega(t) \simeq \sum_{n=1}^{\infty} \beta_n(\Omega)t^{\frac{n}{2}}$

iii. Obtain geometrical information of Ω from β_n

a. area

b. length

c. scalar Curvature

d. mass

e. etc.

D. Conclusion

i. Strengthness

a. Instead of calcualting a complete sequence of the Dirichlet eigenvalues for exploring the shape attributes of a geometry, the asympotoic expansion of the heat content, defined as the integration of the solution to the heat equation over the space-dimension, also implies the geometrical characterisitics.

ii. Limitations

  a. Either irregular geometries or discontinuities lead to the complexities, so the explicit solutions $u(\boldsymbol{s}, t)$ are close to non-existed.

  b. Similiarly, only the first few coeffients β_n in the asymptotic expansion of $Q_\Omega(t)$ can be expressed in the complicated explicit forms.

  c. The numerical evaluation of the analytical $u(\boldsymbol{s}, t)$ and $Q_\Omega(t)$ is usually by no means trivial because they are in the form of infinite series.

III. Numerical Methods for Solving Parabolic Partial Differential Equations

A. Parabolic PDEs: to characterize time-dependent phenomena

B. The intrinsically similar features of the traditional computational techniques are mesh discretization in time and space.

C. Finite Difference Method (FDM) [9]

   i. Basic Ideas: replace derivatives in the equation by the difference quotients;

   ii. A simpliest example of FDM in solving $2-$dimensional heat equation by Forward Time Centered Space (FTCS) [14]

      a. It is an explict method: utilize a simple explicit formula to evaluate the unknown function at each of the spatial mesh points at the new time level.

      b. Prilimarty step: discretize the domain by a set of mesh points.

      c. Secondary step: replace the derivatives by finite difference approximations based on FTCS.

         - discretizes the Laplace operator in space
         - discretizes the time derivative

      d. Third step: determine the time and step size by a condition for numerical stability.

      e. Fourth step: fill in the initial and boundary values in the initialied matrix.

      f. Fifth step: estimate the field values (i.e. tempreature) at the finite number of space-time points by the iterations.

      g. Final Step: visualize the numerical results.

   iii. Stengthness

      a. Compared with other numerical methods, it is the easy to code from the implementational point of view.

   iv. Weakness [3] [10]

      a. The truncation error appears in the process of ignoring the higher-order terms in the Taylor series to obtain the finite difference equations.

      b. Round-off error results from the loss of precision due to the computer rounding of decimal quantities.

      c. Discretization error can be reduced by decreasing the time size, grid size, or both of them, but the computaional time will be longer.

      d. It will be inaccurate and arduous in the practical application when the problem is defined in the irregular geometries.

D. Finite Element Method (FEM) [18]

   i. Foundamental Concepts

a. Finite element: divide the complicated geometries, irregular shapes, and boundaries into an union of smaller and simpler subdomains (e.g. lattice, triangle, curvilinear polygons, etc.) [13]; adjacent element are connected by the nodes.

b. Element equation: reprsent each subdomain by the piecewise continuous polynomial basis function.

c. Model the whole system: assemble all the element equations into a system of algebraic equations.

d. Slove algebraic equations by minimizing the associated error function.

ii. Stengthness

a. Solve a wide range of PDEs defined in a complex geometry.

b. Spatial discretisation is flexible since the mesh can adapt to irregularly shaped boundaries to reduce geometric errors.

c. A specific region can be refined locally to give more resolution.

d. For a considerable number of elements, the parallelling computation can be used to approximate the solution numerically.

iii. Weakness

a. Users may make mistakes in building the FE model, checking the result, detecting and updating the model design.

b. The round-off errors will affect the precision of the nuemrical results.

c. FEM demands a longer execution time and an enormous amount of input data compared with FDM

E. Other Tranditional Computational Methods

i. Finite Volume Method (FVM) [5]

ii. Boundary Element Method (BEM) [1]

F. Limitation in Practice

i. The size of the mesh, subdomain, or volumn will determine the precision of the approximated solution, the smaller being the better. However, the finer discretization will increase the demand for computational resources such as memory and processor time.

ii. In this thesis, the problem domain Ω is bounded by the border of the image and the edge of the whole extremly complicated root system with millions of pixels and various boundary conditions. The complexity of coding is the main practicial limitation.

iii. Approxiating $Q_\Omega(t)$, defined as an integration over the space dimension, results in the extra effort and errors.

IV. Monte Carlo Simulation for Approximating Heat Content $Q_\Omega(t)$

A. Monte Carlo Integration

i. Introduction

a. Definition: utilizing the random sampling of a function to compute an estimate of its integral numerically.

b. Commonly Used Sampling Methods

- Uniform sampling: random points are distributed uniformly in the domain.
- Stratified sampling: splitting up the original integral into a sum of intgrals over sub-regions.
- Importance sampling: choosing samples from a distribution, which has a similar shape as the function being integrated.

ii. Multidimensional Integration

a. General solution $u(\boldsymbol{s}, t) = \int_\Omega C_\Omega(\boldsymbol{s}, t|\boldsymbol{s_0})\delta(\boldsymbol{s} - \boldsymbol{s_0})d\boldsymbol{s_0}$

- Background
  - Stochastic process
  - Brownion motion
    * It is a stochastic process.
    * General definition and history: irregualer, continuous, and permanent random motion observed by Brownion: i.e. microscopic pollen grains suspend in the water.
    * Mathematical definition and properties
  - Stochastic Differential Equations (SDEs)
- Local Solution $u(\boldsymbol{s_0}, t)$
  - Generating a large number of samples starting from $\boldsymbol{s_0}$, which is distributed uniformly within Ω.
  - $u(\boldsymbol{s_0}, t)$ can be expressed as an expecation depending on the sample paths of the stochastic process, i.e. Brownian motion. The sample paths are solutions to the SDEs.
  - Independent random sample trajectories of the stocahstic process can be generated by Monte Carlo techniques to approximate the expectation and thus to estimate $u(\boldsymbol{s_0}, t)$.
- Approximate the global solution $u(\boldsymbol{s}, t)$ by estimating the lacal solution at a large number of points distributed uniformly within Ω.

b. Heat content $Q_\Omega(t) = \int_\Omega u(\boldsymbol{s}, t)d\boldsymbol{s}$

- Sample N points uniformly within Ω.
- $Q_\Omega(t) \approx |\Omega|\frac{1}{N}\sum_{i=1}^{N} u(\boldsymbol{s_i})$

B. Fokker-Planck Equation

   governs the time evolution of the probability density of the Brownian partricles.

C. Monte Carlo Simulation for Diffusing Particels: Lattice Random Walks

   i. Background

      a. Connection Between LRWs and Heat Equation

   ii. Algorithm of LRWs

   iii. Methods for Sample Size Determination

D. Output Analysis

   i. Kaplan-Meier Estimator

   ii. Confidence Interval

   iii. Scaling Relationship

   iv. Two-Sample Statistical Tests

   v. Averaging samples of the fuction at uniform random points within the interval.

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