Walking On Stars

Grid-less Monte Carlo PDE Solver

(SIG Reading Group)

Sept. 27, 2024 Yuqi Meng 1. Spherical Process for the Dirichlet Problem

Definition (Harmonic Function)

A twice continuously differentiable \mathbb{R} -valued function $u:D\to\mathbb{R}$ is **harmonic** if $\Delta u:=\nabla^2 u\equiv 0$ on U.

Definition (Dirichlet Problem)

Given a domain (for simplicity assume that this is simply-connected) D with boundary ∂D , a **Dirichlet problem** associated to a function f continuously defined on ∂D is to find the function u defined on R s.t. u and f coincide on ∂D , i.e. solve for u s.t.

$$\begin{cases} \Delta u = 0, & \text{on D} \\ u|_{\partial D} = f & \text{(Dirichlet BC)} \end{cases}$$

Definition (Brownian Motion)

A \mathbb{R}^d -valued Brownian motion starting at $x \in \mathbb{R}^d$ is a stochastic process $\{B(t) \mid t \in T := \mathbb{R}_{\geq 0}\}$ satisfying the following properties:

- **1** Anchor: B(0) = x.
- ② Independent incrementals: for any increasing sequence $(t_n)_{n \in \mathbb{Z}_{\geq 0}}$ on T, $\{B(t_{i+1}) B(t_i) \mid i \in \mathbb{Z}_{\geq 0}\}$ are independent random variables.
- ③ Normality in each step: For all $t \ge 0$, h > 0, the incremental B(t+h) B(t) follows a normal distribution N(0,h).
- **4** Continuity: The function $t \mapsto B(t)$ is almost surely (i.e., has probability 1 of being) continuous.

Theorem (Kakutani, 1944)

Given a Dirichlet problem defined on a domain D with boundary values $f(\zeta)$ for $\zeta \in \partial D$, for any $x_0 \in D$, the solution u of the Dirichlet problem evaluates to

$$u(x_0) = \int_{\partial D} \Pr(x_0, \zeta, D) f(\zeta) d\zeta \quad \forall x_0 \in D$$

where $\Pr(x_0, \zeta, D)$ is the probability density function of a Brownian motion starting at x_0 intersects for the first time with ∂D at ζ .

Definition (Harmonic Measure)

The measure $d\omega = \Pr(x_0, \zeta, D)d\zeta$ on ∂D is the **harmonic measure**.

First verify the simple case, and then extend to general ones:

• For unit disc, notice that harmonicity is equivalent to "mean value property":

$$f(x) = \frac{1}{\left|\partial S(x,r)\right|} \int_{\partial S(x,r)} f(\zeta) d\zeta$$

where S(x, r) is a sphere centered at x with radius r.

2 Then, use the "local memory-less" property of Brownian motion to extend to arbitrary closed (nice) domains.

Definition (Maximum Sphere)

Let D be an arbitrary domain, and $x \in D$ be an arbitrary point. Then the **maximum sphere** centered at x in D, denoted $K_D(x)$, is the sphere

$$S(x, \inf_{x_0 \in \partial D} \{\|x - x_0\|\})$$

Its boundary (surface of the sphere) is denoted as $\overline{K}_D(x)$.

Definition (Spherical Process (Muller, 1956))

Given a domain D with boundary ∂D and an arbitrary point $x \in D$, the **spherical process** defines a sequence of points $P_n(x, \phi)$ where ϕ is the random variable, as follows:

- **1** $P_0(x, \phi) := x$.
- ② For all $i \in \mathbb{Z}_{\geq 1}$, designate P_i uniformly randomly from $\overline{K}_D(P_{i-1})$.

Notice, that every Brownian motion corresponds to a unique spherical process, and vice versa.

- ⇒: Simply record the position where the given Brownian motion for the first time escapes the maximum sphere.
- The sphere process terminates with probability 0. Therfore they coincide on (countably) infinite points, and the corresponding time.

The argument is flawed with discussion on infinity (but does not interfere with integration).

Definition (Monte Carlo Estimator)

Given a Lebesgue-integrable function $f: D \to \mathbb{R}$, the **Monte Carlo** estimator for the integral

$$I := \int_D f(x) \mathrm{d}x$$

is the sum

$$\hat{I}_N := \frac{1}{N} \sum_{i=1}^N \frac{f(x_n)}{p(x_n)}, \qquad x_{(\cdot)} \sim p(\cdot)$$

Notice that elementary implementation converges slowly. Cf. bidirectional path tracing for reusing paths.

2. Generalizing the Equation

Definition

Given an (ordinary/partial) differential equation with domain Ω ,

- A Dirichlet boundary condition fixes the value of solution on the boundary of domain.
- A Neumann boundary condition fixes the derivative (normal) applied at the boundary of the domain.
- A **Robin boundary condition** is a weighed combination of the previous two. Explicitly, for given *functions a, b, g* defined on $\partial\Omega$ the associated Robin boundary condition is (for target function f)

$$a f + b \partial_n f = g$$
 on $\partial \Omega$

where $\partial_n(\cdot)$ denotes the normal derivative.

Definition (Green Function)

Given a domain D with boundary ∂D , and a differential operator \mathcal{L} , the corresponding **Green function** $G_x^D(y)$ is defined as the solution to the system

$$\mathcal{L}G_{x}^{D}(y)=\delta_{x}(y)$$

where δ_x is the dirac delta function with impulse at x.

Definition (Poisson Kernel)

Under the same setting, the **Poisson kernel** is the normal derivative of *D*:

$$P_x^D(y) := \frac{\partial G_x^D(y)}{\partial n_y}$$

where n_v is the normal vector towards the boundary.

The system then becomes (without Robin BC):

$$\begin{cases} \Delta(u) = f, & \text{on } \Omega & \text{(Poisson)} \\ u = g, & \text{on } \partial\Omega_D & \text{(Dirichlet)} \\ \frac{\partial u}{\partial n} = h, & \text{on } \partial\Omega_N & \text{(Neumann)} \end{cases}$$

Integrating and expressing in weak form gives

$$u = \int_{\partial D} P_x^D(z)g(z)dz \qquad \qquad \text{(Dirichlet)}$$

$$-\int_{\partial D} G_x^D(z)\frac{\partial u(z)}{\partial n_z}dz \qquad \qquad \text{(Neumann)}$$

$$+\int_{D} G_x^D(z)f(z)dz \qquad \qquad \text{(Poisson)}$$

For the case of sphere, $G_x^D \equiv 0$, $P_x^D \equiv \frac{1}{\partial B}$. Further setting $f \equiv 0$ we obtain the result by Kakutani:

$$u = \int_{\partial D} \left(\frac{1}{|\partial D|} \right) g(z) dz$$

Extending from Dirichlet BC for the Dirichlet problem to arbitrary BC for any PDE, the algorithm needs to be modified in the following aspects:

- Generalize Kakutani's principle, taking into consideration of arbitrary differential operators.
- Use different boundary treatments (for Dirichlet BC, this is just terminating the walk).
- Generalize the Spherical Process to ensure convergence.

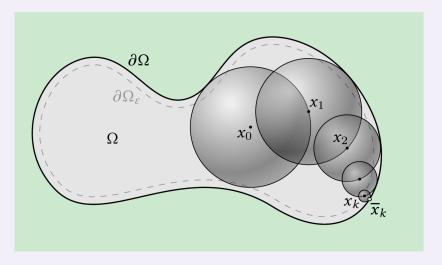
3. Boundary Treatments

Think in terms of rendering, we have the natural analogy of BCs:

- 1 Dirichlet BC fixes the value, can be regarded as the *light source*.
- Neumann BC fixes the normal derivative, can be regarded as reflection.
- 3 Robin BC mixes the two above, can be regarded as the specular/diffusion coefficient.

This naturally inspires the following treatment (rigorous proof will not be simple).

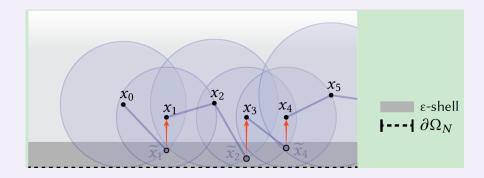
Following the previous reduction to spherical process, the Monte Carlo integrator terminates at Dirichlet BCs:



Notice: Neumann BC alone cannot fix a solution.

The intuitive approach would be to let sample points "bounce back" in the normal direction to only capture the tangential component.

However, this will cause instabilities...



Change: set radius to minimum of distance to Dirichlet boundary, and distance to "silhouette" points:

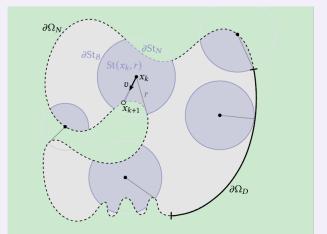
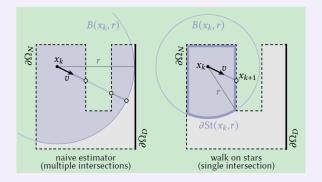


Fig. 8. We use star-shaped regions defined by intersecting a ball $B(x_k,r)$ with the domain Ω and taking the component connected to x_k . The ball does not contain the Dirichlet boundary $\partial\Omega_D$: only visible parts of the Neumann boundary $\partial\Omega_N$ and the spherical part of ∂B .

The silhouette points are defined to avoid divergence:



Radius update is set in random direction, and intersection with Neumann part first, then spherical part.

Many intricate details here.

Natural thought: blend between Dirichlet BC and Neumann BC.

High level idea: mimic the solution to path tracing. Interpolate between the radius for pure Dirichlet and pure Neumann for radius update, and apply Russian Roulette for early termination. This is possible as Robin BC contains information about Dirichlet BC.

Foundation:

Monte Carlo Geometry Processing: A Grid-Free Approach to PDE-Based Methods on Volumetric Domains (2020) Subsequent Works:



Thank you!