WALK ON SPHERES ALGORITHMS FOR HELMHOLTZ AND LINEARIZED POISSON-BOLTZMANN EQUATIONS

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Abstract

We show that a constant-potential time-independent Schrödinger equation with Dirichlet boundary data can be reformulated as a Laplace equation with Dirichlet boundary data.

With this reformulation, which we call the Duffin correspondence, we provide a classical Walk On Spheres algorithm for Monte Carlo simulation of the solutions of the said boundary value problem.

Outline

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Preliminaries

Let $x = (x_1, \ldots, x_n)$. Denote

$$\Delta_x = \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2}$$

We consider the Dirichlet-type boundary value problem of the Schrödinger equation with constant potential $\lambda \in \mathbb{R}$:

$$\begin{cases} \frac{1}{2}\Delta_x u(x) - \lambda u(x) = 0 & \text{on } x \in D, \\ u(y) = f(y) & \text{on } y \in \partial D. \end{cases}$$

Here D is a domain and f is (continuous and) bounded on ∂D. The case $\lambda > 0$ corresponds to the Yukawa equation, or the linearized Poisson–Boltzmann equation. The case $\lambda = 0$ is the Laplace equation. The case $\lambda < 0$ is the Helmholtz equation.

Preliminaries

Conditions for the domain D of a Helmholtz–Yukawa problem to admit a unique bounded (strong) solution are best expressed by using probabilistic tools:

Let W be the n-dimensional Brownian motion, i.e., the unique Markov process with the generator $\frac{1}{2}\Delta_x$.

Let

$$\tau_D = \inf\{t > 0\,;\, W_t \notin D\}.$$

Let $\mathbf{P}^x$ denote the probability measure under which $W_0 = x$.

Preliminaries

Assumptions

1. The domain D is *Wiener regular*, i.e.,

$$\mathbf{P}^y[\tau_D = 0] \quad \text{for all } y \in \partial D.$$

2. The domain D is *Wiener small*, i.e.,

$$\mathbf{P}^x[\tau_D < \infty] = 1 \quad \text{for all } x \in D.$$

3. Finally, we assume that the domain D is *gaugeable*, i.e.,

$$\sup_{x \in D} \mathbf{E}^x \left[e^{-\lambda \tau_D} \right] < \infty.$$

Preliminaries

1. All domains with piecewise C^1 boundary are Wiener regular.
2. If any projection of the domain D on any subspace $\mathbb{R}^{n'}$, $n' \leq n$ is bounded, then D is Wiener small.
3. The gauge condition is satisfied if

$$\lambda > -\frac{1}{2}\mathrm{Leb}(D)^{-2/n}\left(\frac{\pi^{n/2}}{\Gamma(n/2+1)}\right)^{2/n} j^2_{n/2-1,1}.$$

Proposition (Stochastic representation)

The Helmholtz–Yukawa equation admits the bounded solution

$$u(x) = \mathbf{E}^x\left[e^{-\lambda\tau_D} f\left(W_{\tau_D}\right)\right].$$

Outline

Duffin correspondence

Set $\bar{x} = (x, x') \in \mathbb{R}^n \times \mathbb{R}$ and

$$
\begin{aligned}
g(\lambda; x') &= \begin{cases} \cos\left(\sqrt{2\lambda}\, x'\right), & \text{for } \lambda > 0, \\ \cosh\left(\sqrt{-2\lambda}\, x'\right), & \text{for } \lambda < 0. \end{cases}, \\
I(\lambda) &= \begin{cases} \left(-\frac{\pi}{2\sqrt{2\lambda}}, \frac{\pi}{2\sqrt{2\lambda}}\right), & \text{for } \lambda > 0, \\ \mathbb{R}, & \text{for } \lambda < 0, \end{cases} \\
\bar{D}(\lambda) &= D \times I(\lambda), \\
\bar{u}(\lambda; \bar{x}) &= u(x) g(\lambda; x'), \\
\bar{f}(\lambda; \bar{y}) &= f(y) g(\lambda; y').
\end{aligned}
$$

$$
\begin{cases} \frac{1}{2}\Delta_{\bar{x}} \bar{u}(\lambda; \bar{x}) = 0 & \text{on } \bar{x} \in \bar{D}(\lambda), \\ \bar{u}(\lambda; \bar{y}) = \bar{f}(\lambda; \bar{y}) & \text{on } \bar{y} \in \partial \bar{D}(\lambda). \end{cases}
$$

Duffin correspondence

Theorem (Duffin correspondence)

u is the bounded solution to the Helmholtz–Yukawa equation iff $\bar{u}$ is the bounded solution to the Laplace equation.

Let $\bar{W} = (W, W')$ be an $(n+1)$-dimensional Brownian motion and let $\tau_{I(\lambda)} = \inf\{t > 0\,;\ W'_t \notin I(\lambda)\}$.

Corollary (Simple stochastic representation)

The Helmholtz–Yukawa equation admits the bounded solution

$$u(x) = \mathbf{E}^{x,0}\left[f\left(W_{\tau_D}\right) g\left(\lambda; W'_{\tau_D}\right)\ ;\ \tau_{I(\lambda)} > \tau_D\right].$$

Outline

Denote

$$\begin{aligned} \tau_x &= \inf\{t > 0\,;\ W_t \notin D\}\,, \\ \tau'_{x'} &= \inf\left\{t > 0\,;\ W'_t \notin I(\lambda)\right\}\,, \\ \bar\tau_{\bar x} &= \inf\left\{t > 0\,;\ \bar W \notin \bar D(\lambda)\right\}\,. \end{aligned}$$

Note that τ_x and $\tau'_{x'}$ are independent, and $\bar\tau_{\bar x} = \min\left(\tau_x, \tau'_{x'}\right)$.

For $x \in D$, denote $\bar x = (x, 0) \in \bar D(\lambda)$.

The stochastic approximation for $u(x)$ is

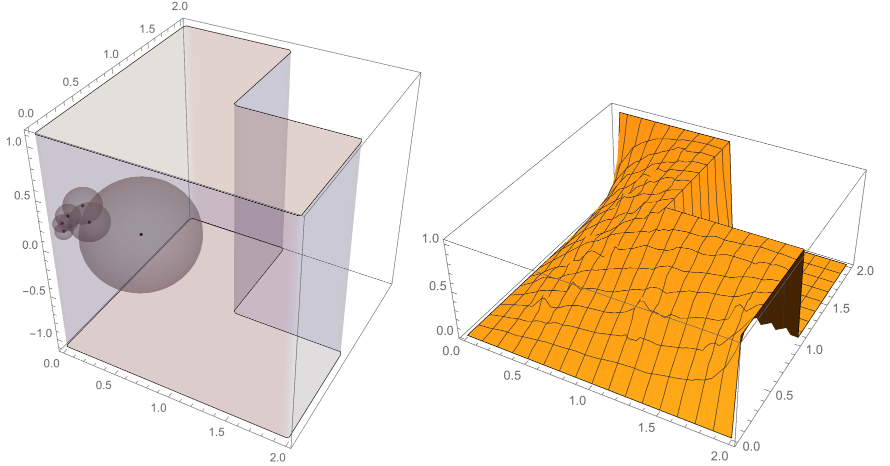
$$\hat u_K(x) = \frac{1}{K}\sum_{k=1}^{K} \bar f\left(\lambda\,;\ \bar w^k_{\bar x}\left(\bar\tau^k_{\bar x}\right)\right).$$

Here$\bar\tau^k_{\bar x}$ is the termination-step of the trajectory k. The trajectories are generated by the following DWOS Algorithm:

Algorithm (DWOS)

Fix a small parameter $\varepsilon > 0$.

1. Initialize: $\bar{w}_{\bar{x}}(0) = (w_x(0), (w')_0(0)) = (x, 0)$.
2. While $\mathrm{dist}(\bar{w}_{\bar{x}}(j), \partial \bar{D}(\lambda)) > \varepsilon$:
    1. Set $r(j) = \mathrm{dist}(\bar{w}_{\bar{x}}(j), \partial \bar{D}(\lambda))$.
    2. Sample $\xi(j)$ independently from the unit sphere $\partial B_{n+1}(0,1)$.
    3. Set $\bar{w}_{\bar{x}}(j+1) = \bar{w}_{\bar{x}}(j) + r(j)\xi(j)$.
3. When $\mathrm{dist}(\bar{w}_{\bar{x}}(j), \partial \bar{D}(\lambda)) \leq \varepsilon$:
4. Set $\mathrm{pr}\, \bar{w}_{\bar{x}}(j)$ to be the orthogonal projection of $\bar{w}_{\bar{x}}(j)$ to $\partial \bar{D}(\lambda)$.
5. Return $\mathrm{pr}\, \bar{w}_{\bar{x}}(j)$.



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Suppose we want use the WOS algorithm directly without the Duffin correspondence. To do this, we must estimate the term $e^{-\lambda\tau_D}$. Suppose the WOS algorithm takes T steps to hit the boundary with balls of radii $r_1, r_2, \ldots, r_T$. The Weighted Walk On Spheres (WWOS) algorithm is based on the fact that the term $e^{-\lambda\tau_D}$ can be decomposed into independent terms

$$e^{-\lambda\tau_D} = e^{-\lambda\tau_{r_1}} e^{-\lambda\tau_{r_2}} \cdots e^{-\lambda\tau_{r_T}},$$

where the τ_{r_j}'s are the exit times of the Brownian motion from balls of radius r_j, and these exit times are also independent of the exit locations from the ball. Consequently, at each step j of the WOS algorithm, the Brownian particle gains (or loses) an independent multiplicative weight that is given by

$$\mathbf{E}^{W_{\tau_{j-1}}} \left[e^{-\lambda\tau_{r_j}} \right] = \mathbf{E}^0 \left[e^{-\lambda\tau_{r_j}} \right].$$

By using the 1/2-self-similarity of the Brownian motion we see that

$$\mathbf{E}^0\left[e^{-\lambda\tau_r}\right] = \mathbf{E}^0\left[e^{-\lambda r^2\tau_1}\right] = \psi(\lambda r^2).$$

For $\mu > 0$ the function ψ is well-known:

$$\psi(\mu) = \begin{cases} \frac{\mu^\nu}{2^\nu\Gamma(\nu+1)I_\nu(\mu)}, & n = 2\nu - 2 \geq 2, \\ \frac{1}{\cosh(\sqrt{2\lambda})}, & n = 1. \end{cases}$$

For $\mu < 0$, as far as we know, no simple formula for $\psi(\mu)$ is known. However, the distribution function of τ_1 is well-known:

$$\mathbf{P}^0\left[\tau_1 \leq t\right] = 1 - \frac{1}{2^{\nu-1}\Gamma(\nu+1)}\sum_{i=1}^{\infty}\frac{j_{\nu,i}^{\nu-1}}{J_{\nu+1}(j_{\nu,i})}\exp\left\{-\frac{1}{2}j_{\nu,i}^2\, t\right\},$$

where $j_{\nu,i}$'s are the positive zeros J_ν in the increasing order.

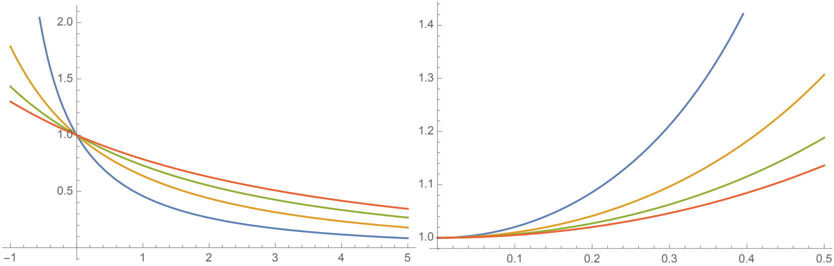

Figure : The function $\psi(\lambda)$ for $\lambda \in (-1, 5)$ for $n = 1, 2, 3, 4$, where $n = 1$ on the top (left). The function $\psi(-2r^2)$, $r > 0$, where the dimension are $n = 1, 2, 3, 4$, where $n = 1$ on the top (right).

The approximation for $u(x)$ is

$$\hat{u}_K(x) = \frac{1}{K}\sum_{k=1}^{K} c_x^k(\lambda) f\left(w_x^k(\tau_x^k)\right).$$

Hereτ_x^k is the exit time for the each individual particle and $c_x^k(\lambda) = e^{-\lambda \tau_x^k}$.

The individual particle exit locations $w_x(\tau_x)$ and weights c_x^k are generated by the following WWOS algorithm:

Algorithm (WWOS)

Fix a small parameter $\varepsilon > 0$.

1. Initialize: $w_x(0) = x$, $c_x(0) = 0$
2. While $\operatorname{dist}(w_x(j), D) > \varepsilon$:
    1. Set $r(j) = \operatorname{dist}(w_x(j), \partial D)$.
    2. Sample $\xi(j)$ independently from the unit sphere $\partial B_n(0,1)$.
    3. Set $w_x(j+1) = w_x(j) + r(j)\xi(j)$ and $c_x(j+1) = c_x(j)\psi(\lambda r(j)^2)$.
3. When $\operatorname{dist}(w_x(j), \partial D) \leq \varepsilon$:
4. Set $\operatorname{pr} w_x(j)$ to be the orthogonal projection of $w_x(j)$ to ∂D.
5. Return $\operatorname{pr} w_x(j)$ and $c_x(j)$.

For the Yukawa case $\lambda > 0$, the weight loss $e^{-\lambda\tau_D}$ of the particle can be interpreted as independent exponential killing of the particle.

Our estimator for $u(x)$ is

$$\hat{u}_K(x) = \frac{1}{K} \sum_{k \in K^*(\lambda)} f(w_x^k(\tau_x^k)),$$

where w_x^k, $k = 1, \ldots, K$ are independent simulations of the trajectories Brownian particles starting from point x, and the set $K^*(\lambda) \subset \{1, \ldots, K\}$ contains the particles that are not killed; τ_x^k is the termination-step time of the algorithm. The individual particles are generated by the following KWOS algorithm:

Algorithm (KWOS)

Fix a small parameter $\varepsilon > 0$.

1. Initialize: $w_x(0) = x$.
2. While $\operatorname{dist}(w_x(j), D) > \varepsilon$:
    1. Set $r(j) = \operatorname{dist}(w_x(j), \partial D)$.
    2. Kill the particle with probability $1 - \psi(\lambda r(j)^2)$. If the particle is killed, the algorithm terminates and returns 0.
    3. Sample $\xi(j)$ independently from the unit sphere $\partial B_n(0, 1)$.
    4. Set $w_x(j+1) = w_x(j) + r(j)\xi(j)$.
3. When $\operatorname{dist}(w_x(j), \partial D) \leq \varepsilon$:
4. Set $\operatorname{pr} w_x(j)$ to be the orthogonal projection of $w_x(j)$ to ∂D.
5. Return $\operatorname{pr} w_x(j)$.

Thank you for listening!

Any questions?