Sphere stepping algorithms for Dirichlet-type problems with the fractional Laplacian

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Walk-on-spheres

- Suppose that D is an open domain in $\mathbb{R}^d$, $d \geq 2$, with sufficiently smooth boundary. We are interested in the existence of twice differentiable solutions to the partial differential equation

$$\begin{aligned} \triangle u(x) &= 0, & u &\in D \\ u(x) &= f(x), & x &\in \partial D, \end{aligned}$$

  where f is a continuous function.
- Feynman–Kac representation: if $u \in C^2(D)$ is a solution iff

$$u(x) = \mathbb{E}_x[f(B_{\tau_D})], \qquad x \in D,$$

  where $\tau_D = \inf\{t > 0 : B_t \notin D\}$ and $B := (B_t, t \geq 0)$ is a standard d-dimensional Brownian motion with probabilities $(\mathbb{P}_x, x \in \mathbb{R}^d)$.

Monte-Carlo approximation

Thanks to the SLLN

$$u(x) = \lim_{n\to\infty} \frac{1}{n} \sum_{i=1}^{n} f(B^{(i)}_{\tau^{(i)}_D})$$

where $(B^{(i)}_t : t \geq 0)$, $i \geq 1$, are iid BMs with $\tau^{(i)}_D = \inf\{t > 0 : B^{(i)}_t \notin D\}$. If e.g. f, D bounded, then rate of convergence is optimal thanks to CLT.

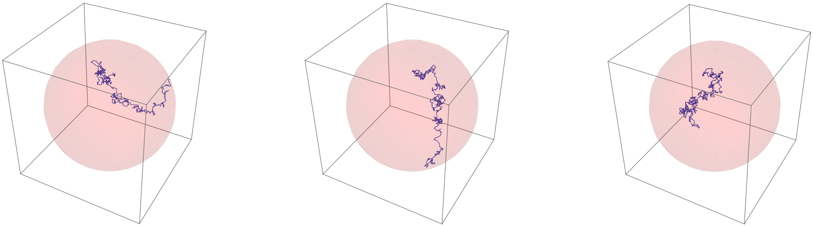


Figure: Images sourced from Wolfram: Here D is the unit sphere.

Walk-on-sphere

- A method proposed by M. Muller in 1956 for the case that D is convex,
- set $\rho_0 = x$ for $x \in D$ and define r_1 to be the radius of the largest sphere circumscribed in D that is centred at x. This sphere we will call $S_1 = \{y \in \mathbb{R}^d : |y - x| = r_1\}$.
- Now set $\rho_1 \in D$ to be a point uniformly distributed on S_1
- Construct the remainder of the sequence $(\rho_n,\ n \geq 1)$ inductively.
- Given ρ_{n-1}, we may define the radius, r_n, of the largest sphere circumscribed in D that is centred at ρ_{n-1}. Calling this sphere S_n, we have that $S_n = \{y \in \mathbb{R}^d : |y - \rho_{n-1}| = r_n\}$. We now select ρ_n to be a point that is uniformly positioned on S_n.

Theorem

We have for all $x = \rho_0 \in D$, $\lim_{n\to\infty} \rho_n \stackrel{d}{=} B_{\tau_D}$.

Walk-on-sphere

- Algorithm never ends, spheres become smaller as algorithm approaches the boundary
- Artificially end algorithm at $N(\varepsilon) = \inf\{n \geq 0 : \sup_{y \in \partial D} |\rho_n - y| < \varepsilon\}$
- Run MC algorithm with $f(\rho_N)$.

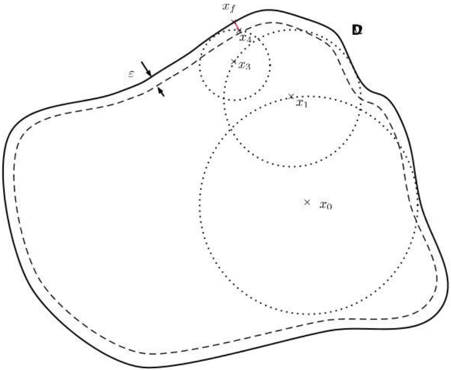


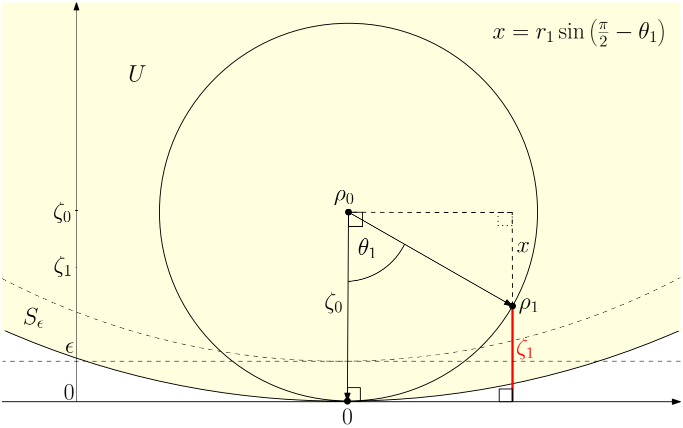
Figure: Sourced from: `https://en.wikipedia.org/wiki/Walk-on-spheres_method`

Rate of convergence

Theorem (Muller 1956/Motoo 1959)

Suppose that D is bounded and convex. There exist constants $c_1, c_2 > 0$ such that $\mathbb{E}_x[N(\epsilon)] \leq c_1 |\log \epsilon| + c_2$, $\epsilon \in (0,1)$.

- Define
$$\zeta_1 = \min\left\{\epsilon, \inf_{z \in \partial V(\rho_0)} |\rho_1 - z|\right\};$$
where $\partial V(\rho_0)$ is the tangent hyperplane of nearest point on ∂D to ρ_0.
- Next, define θ_1, the angle that subtends at ρ_0 between ρ_1 and the closest point on ∂D to ρ_0, recall that symmetry implies that $\theta_1 \sim U[0, 2\pi]$.
- Simple geometric considerations tell us that, on $\{\zeta_1 > \epsilon\}$
$$\zeta_1 = \zeta_0(1 - \cos(\theta_1)).$$
- Note that the event $\{\zeta_1 = \epsilon\}$ corresponds to $\theta_1 \in [-\theta^*(\zeta_0), \theta^*(\zeta_0)]$
$$\theta^*(\zeta_0) = \arccos\left(\frac{\zeta_0 - \epsilon}{\zeta_0}\right).$$
- Simple geometric computations give us
$$\mathbb{E}_{\rho_0}[\sqrt{\zeta_1}] \leq \sqrt{\epsilon}\,\mathbb{P}_{\rho_0}(\theta_1 \in (-\theta^*(\zeta_0), \theta^*(\zeta_0))) + \mathbb{E}_{\rho_0}\left[\mathbf{1}_{(\theta_1 \notin (-\theta^*(\zeta_0), \theta^*(\zeta_0)))}\sqrt{\zeta_1}\right]$$
$$\leq \lambda\sqrt{\zeta_0}, \text{ for some } \lambda \in (0,1)$$



- Sequentially define $(\zeta_n, n \geq 0)$ (writing $\zeta_{n+k} = \epsilon$, $k \geq 1$, if $\zeta_n = \epsilon$) and note $(\lambda^{-n}\sqrt{\zeta_n}, n \geq 0)$ is a supermartingale.
- We have $N(\epsilon) \leq N'(\epsilon) := \min\{n \geq 0 : \zeta_n = \epsilon\}$.
- Jensen's inequality gives us, for $\rho_0 = x \in D$,

$$\epsilon\lambda^{-\mathbb{E}_x[N'(\epsilon)]} \geq \mathbb{E}_x[\lambda^{-N'(\epsilon)}\epsilon] \leq \sqrt{\zeta_1}.$$

The result now follows by taking logarithms.

Dirichlet problem for the fractional Laplacian

- The Dirichlet problem for fractional Laplacian $-(-\triangle)^{\alpha/2}$, $\alpha \in (0, 2)$, requires one to find a solution to the system

$$\begin{aligned} -(-\triangle)^{\alpha/2} u(x) &= 0, \qquad && u \in D, \\ u(x) &= f(x), && x \in D^{\mathrm{c}}, \end{aligned}$$

  where f is a suitably regular function.
- In dimension two or greater, up to a multiplicative constant,

$$-(-\triangle)^{\alpha/2} u(x) = -\frac{\Gamma((d+\alpha)/2)}{2^{\alpha}\pi^{d/2}\Gamma(-\alpha/2)} \lim_{\epsilon \downarrow 0} \int_{\mathbb{R}^d \setminus B(0,\epsilon)} \frac{[u(y) - u(x)]}{|y - x|^{d+\alpha}} \mathrm{d}y, \qquad x \in \mathbb{R}^d,$$

  where $B(0, \epsilon) = \{x \in \mathbb{R}^d : |x| < \epsilon\}$ and u is smooth enough for the limit to make sense.

Fractional Laplacian

- The Laplacian serves as the infinitesimal generator of Brownian motion, in the sense that, for appropriately smooth functions f,

$$\lim_{t\to 0}\frac{\mathbb{E}_x[f(B_t)]-f(x)}{t}=\frac{1}{2}\triangle f(x), \qquad x\in\mathbb{R}^d.$$

- The fractional Laplacian is similarly related to a stable process, a strong Markov process with stationary and independent increments, say $X=(X_t,t\geq 0)$ with probabilities $(\mathbb{P}_x, x\in\mathbb{R}^d)$, whose semi-group is represented by the Fourier transform

$$\mathbb{E}_0[\mathrm{e}^{\mathrm{i}\langle\theta,X_t\rangle}]=\mathrm{e}^{-|\theta|^\alpha t}, \qquad \theta\in\mathbb{R}^d, t\geq 0,$$

  where $\langle\cdot,\cdot\rangle$ represents the usual Euclidian inner product.
- The stability index $\alpha\in(0,2)$. The case $\alpha=2$ is Brownian motion.
- In a small period of time $[t,t+dt]$, the process will experience a discontinuity, say $(\Delta|x|,\Delta\mathrm{Arg}x)=(r,\theta)$ with probability

$$C\left(\frac{1}{r^{1+\alpha}}\sigma(\mathrm{d}\theta)\mathrm{d}r\right)\mathrm{d}t+o(\mathrm{d}t),$$

  where C is a constant and $\sigma(\mathrm{d}\theta)$ is the uniform measure on $\mathbb{S}_{d-1}$.

Three special properties of stable processes like Brownian motion

- **Spatial homogeneity:** We have for any $x \in \mathbb{R}^d$,

$$((X_t - x, t \geq 0), \mathbb{P}_x) \text{ is equal in law to } ((X_t, t \geq 0), \mathbb{P}_0).$$

- **Scaling:** For α-stable Lévy processes, we have the following important scaling property: for all $c > 0$,

$$((cX_{c^{-\alpha}t}, t \geq 0), \mathbb{P}_0) \text{ is equal in law to } ((X_t, t \geq 0), \mathbb{P}_0).$$

- **Rotational invariance:** Suppose that U corresponds to a rotation in space, then

$$((UX_t, t \geq 0), \mathbb{P}_x) \text{ is equal in law to } ((X_t, t \geq 0), \mathbb{P}_{Ux}).$$

Solving Dirichlet problem for the fractional Laplacian

For any function f on $\mathbb{R}^d$, we say it belongs to $L^1_\alpha(\mathbb{R}^d)$ if it is a non-negative measurable function that satisfies

$$\int_{\mathbb{R}^d} \frac{f(x)}{1+|x|^{\alpha+d}} \mathrm{d}x < \infty.$$

Theorem

For dimension $d \geq 2$, suppose that D is a bounded convex domain in $\mathbb{R}^d$ and that f is a non-negative continuous in $L^1_\alpha(\mathbb{R}^d)$. Then there exists a unique continuous solution to the Dirichlet problem for fractional Laplacian in $L^1_\alpha(\mathbb{R}^d)$, which is given by

$$u(x) = \mathbb{E}_x[f(X_{\sigma_D})], \qquad x \in D,$$

where $\sigma_D = \inf\{t > 0 : X_t \notin D\}$.

Stable walk-on-spheres

- What happens to the walk-on-spheres approach for stable processes?
- Stable processes exit spheres by a jump and hence one can no longer select the exit point uniformly on the boundary of the sphere, but from an isotropic distribution on the complement of the sphere.

Theorem (Blumenthal, Getoor, Ray, 1961)

Suppose that $B(0,1)$ is a unit ball centred at the origin and write $\sigma_{B(0,1)} = \inf\{t > 0 : X_t \notin B(0,1)\}$. Then,

$$\mathbb{P}_0(X_{\sigma_{B(0,1)}} \in \mathrm{d}y) = \pi^{-(d/2+1)}\,\Gamma(d/2)\,\sin(\pi\alpha/2)\,\left|1 - |y|^2\right|^{-\alpha/2} |y|^{-d}\,\mathrm{d}y,$$

for $|y| > 1$.

- Scaling allows us to convert this result to give the exit distribution for a sphere of any radius.
- The algorithm no longer needs to be stopped on approaching an ϵ-skin, can now work with

$$N = \inf\{n \geq 0 : \rho_n \notin D\}.$$

Super fast sampling

Theorem

Suppose that D is convex (does not need to be bounded). For all $x \in D$, there exists a constant $p = p(\alpha, d) > 0$ (independent of x) and a random variable Γ such that $N \leq \Gamma$ almost surely, where

$$\mathbb{P}(\Gamma = k) = (1-p)^{k-1}p, \qquad k \in \mathbb{N}.$$

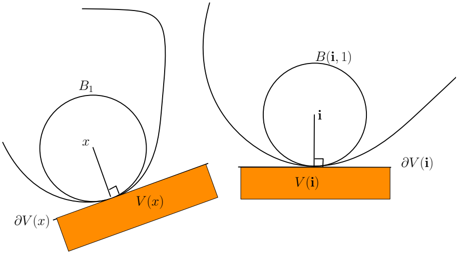
Or said another way,

$$\mathbb{P}_x(N > n) \leq \mathbb{P}(\Gamma > n) = (1-p)^n$$

Proof of Theorem

- Scaling and spatial homogeneity tells us:

$$X^{(x)}_{\sigma_{B_1}} - x =^d |x|(X^{(\mathbf{i})}_{\sigma_{B(\mathbf{i},1)}} - \mathbf{i}),$$



- Define

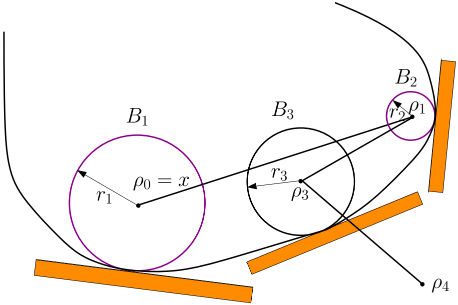
$$I_D(x) = \mathbf{1}_{\{X^{(x)}_{\sigma_{B_1}} \notin D\}} \quad \text{and} \quad I_V(x) = \mathbf{1}_{\{X^{(x)}_{\sigma_{B_1}} \in V(x)\}}.$$

Then $I_D(x) \geq I_V(x)$ and, independently of $x \in D$, $\mathbb{P}(I_V(x) = 1) = p(\alpha, d)$, where

$$p(\alpha, d) := \mathbb{P}_{\mathbf{i}}(X_{\sigma_{B(\mathbf{i},1)}} \in V(\mathbf{i})) = \frac{\Gamma(d/2)}{\pi^{(d+2)/2}} \sin(\pi\alpha/2) \int_{x_1<-1} \left|1 - |x|^2\right|^{-\alpha/2} |x|^{-d} \, dx.$$

Proof of Theorem

- Compare each step of the algorithm with exiting the scaled ball into the tangent hyperplane and this gives the stochastic upper bound by a geometric random variable whose distribution does not depend on x.



Non-convex domains

Definition

A domain D in $\mathbb{R}^d$ is said to satisfy the *uniform exterior-cone condition*, henceforth written UECC, if there exist constants $\eta > 0$, $r > 0$ and a cone

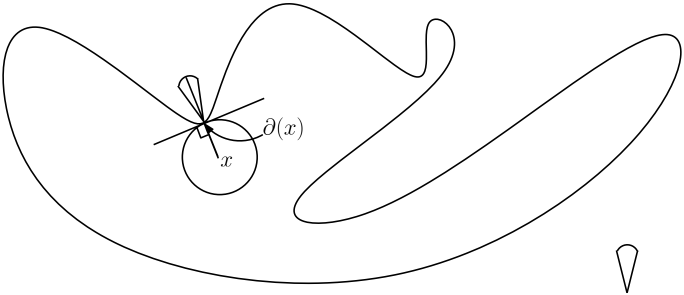
$$\mathrm{Cone}(\eta) = \{x = (x_1, \cdots, x_d) \in \mathbb{R}^d : |x| < \eta x_1\}$$

such that, for every $z \in \partial D$, there is a cone C_z with vertex z, isometric to $\mathrm{Cone}(\eta)$ satisfying $C_z \cap B(z, r) \subset D^c$.

We say that D satisfies the *regularised uniform exterior-cone condition*, written RUECC, if it is UECC and the following additional condition holds: for each $x \in D$, suppose that $\partial(x)$ is a closest point on the boundary of D to x. Then the isometric cone that qualifies D as UECC can be placed with its vertex at $\partial(x)$ and symmetrically oriented around the line that passes through x and $\partial(x)$.

- It is well known that, for example, bounded $C^{1,1}$ domains satisfy (UECC). We need a slightly more restrictive class of domains than those respecting UECC.

Non-convex domains



Theorem

Suppose that D is bounded and satisfies RUECC. Then, for each $x \in D$, there exists a random variable $\hat{\Gamma}$ such that $N \leq \hat{\Gamma}$ almost surely and

$$\mathbb{P}(\hat{\Gamma} = k) = (1 - \hat{p})^{k-1}\hat{p}, \qquad k \in \mathbb{N},$$

for some $\hat{p} = \hat{p}(\alpha, D)$.

Non-convex domains: only openness and boundedness

Theorem

Suppose that D is open and bounded. Then for all $x \in D$, there exists a constant $q_\epsilon = q_\epsilon(\alpha, D) > 0$ (independent of x) and a random variable Γ^ϵ such that $N \leq \Gamma^\epsilon$ almost surely, where

$$\mathbb{P}_x(\Gamma^\epsilon = k) = (1 - q_\epsilon)^{k-1} q_\epsilon, \qquad k \in \mathbb{N}.$$

Moreover, $q_\epsilon = \mathcal{O}(\epsilon^\alpha)$ as $\epsilon \downarrow 0$. In particular

$$\mathbb{E}_x[N(\epsilon)] = \mathcal{O}(\epsilon^{-\alpha}), \qquad \text{as } \epsilon \downarrow 0.$$

- In this case, we compare the exit from every sphere in the algorithm against a global sphere which completely surrounds the domain D (and hence we need that it is bounded).

Numerical experiments: $D = B(0,1)$

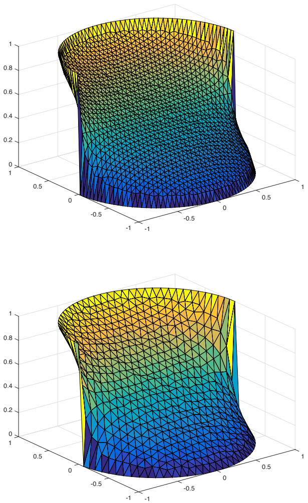


Figure: All four cases consider boundary data $g(x,y) = \mathbf{1}_{(x>0)}$ for different α (in decreasing order).

Numerical experiments: $D = B(0,1)$

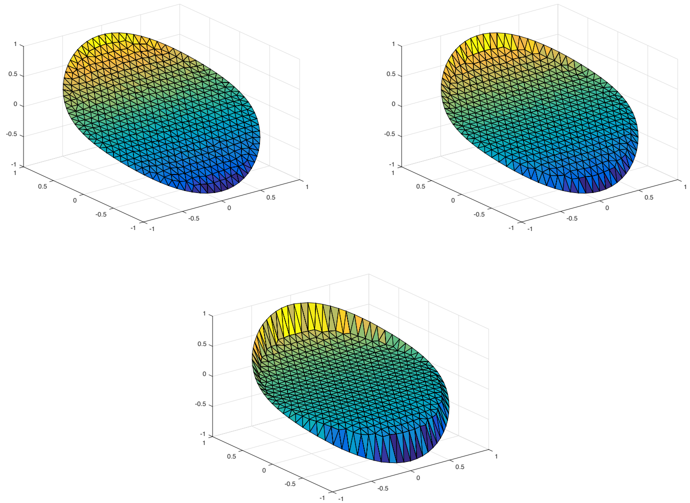


Figure: All three cases consider boundary data $g(x,y) = \cos(x)\sin(y)$ for different α (in decreasing order)

Numerical experiments: Geometric steps

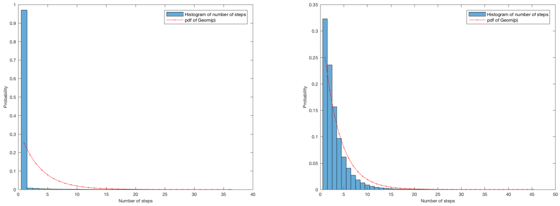


Figure: $x = (0.001, 0.001)$ (left) and $x = (0.6, 0.6)$ (right)

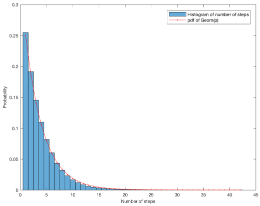


Figure: x very close to the boundary

Numerical experiments: Comparison with exact solution on $D = B(0,1)$

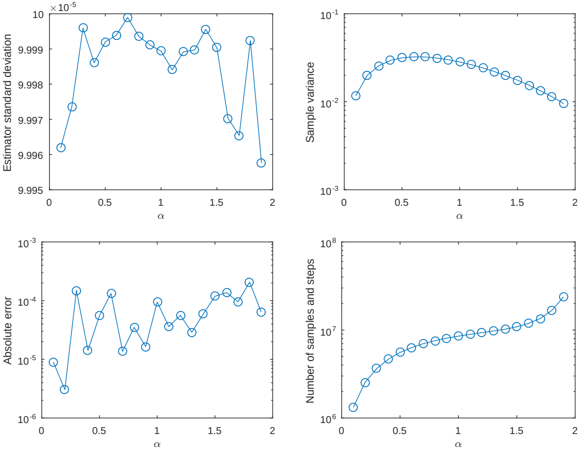


Figure: Example simulation with the walk-on-spheres algorithm based on desired tolerance of 10^{-4}. From top left to bottom right, we see the standard deviation of the estimator, the sample variance, the absolute error (using a quadrature approximation for the integral in Blumenthal-Getoor-Ray formula for the reference value), and the amount work (number of samples $\times$ mean number of steps).

Fractional Poisson problem

- Introduce inhomogeneity

$$\begin{aligned} -(-\triangle)^{\alpha/2}u(x) &= -g(x), \qquad && x \in D, \\ u(x) &= f(x), \qquad && x \in D^{c}, \end{aligned} \tag{1}$$

for suitably regular functions $g\colon D \to \mathbb{R}$ and $f\colon D \to \mathbb{R}$.

Theorem

Let $d \geq 2$ and assume that D is a bounded convex domain in $\mathbb{R}^d$. Suppose that f is a non-negative continuous function which belongs to $L^1_\alpha(\mathbb{R}^d)$. Moreover, suppose that g is a function in $C^{\alpha+\epsilon}(\mathbb{R}^d)$ for some $\epsilon > 0$. Then there exists a unique non-negative continuous solution to (1) in $L^1_\alpha(\mathbb{R}^d)$ which is given by

$$u(x) = \mathbb{E}_x[f(X_{\sigma_D})] + \mathbb{E}_x\left[\int_0^{\sigma_D} g(X_s)\mathrm{d}s\right], \qquad x \in D,$$

where $\sigma_D = \inf\{t > 0 : X_t \notin D\}$.

Fractional Poisson problem

Theorem (Blumenthal, Getoor, Ray 1961)

If we write

$$V_r(x, \mathrm{d}y) := \int_0^\infty \mathbb{P}_x(X_t \in \mathrm{d}y,\ t < \sigma_{B(x,r)})\,\mathrm{d}t, \qquad x \in \mathbb{R}^d,\ |y| < 1,\ r > 0,$$

then

$$V_1(0, \mathrm{d}y) = 2^{-\alpha}\,\pi^{-d/2}\,\frac{\Gamma(d/2)}{\Gamma(\alpha/2)^2}\,|y|^{\alpha-d}\left(\int_0^{|y|^{-2}-1}(u+1)^{-d/2}u^{\alpha/2-1}\mathrm{d}u\right)\mathrm{d}y.$$

- For $x \in D$, using the strong Markov property we have the representation

$$u(x) = \mathbb{E}_x[f(\rho_N)] + \mathbb{E}_x\left[\sum_{n=0}^{N-1} V_1(0, r_n^\alpha g(\rho_n + r_n\cdot))\right]$$

- Hence this suggests the Monte-Carlo algorithm using walk-on-sphere quantities (ρ_n, r_n), $n \le N$,

$$\boxed{f(\rho_N) + \sum_{n=0}^{N-1} r_n^\alpha\, V_1(0, g(\rho_n + r_n\cdot)), \qquad x \in D,}$$

Thank you!