Monte Carlo methods for Solving PDEs
Computational Physics Final Project

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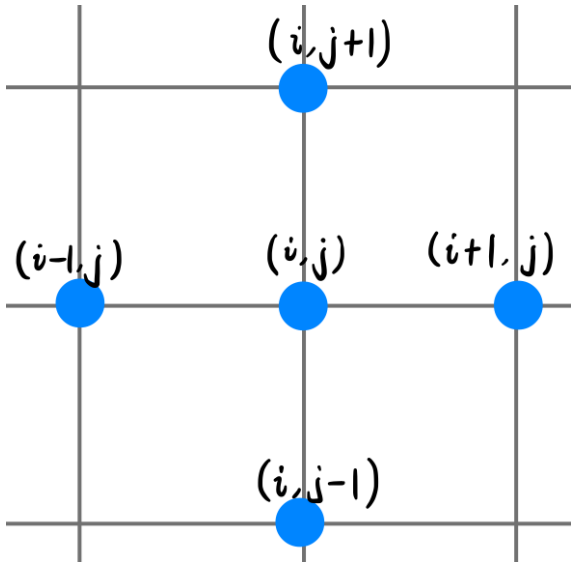
Laplace's Equation with Dirichlet Boundary Condition

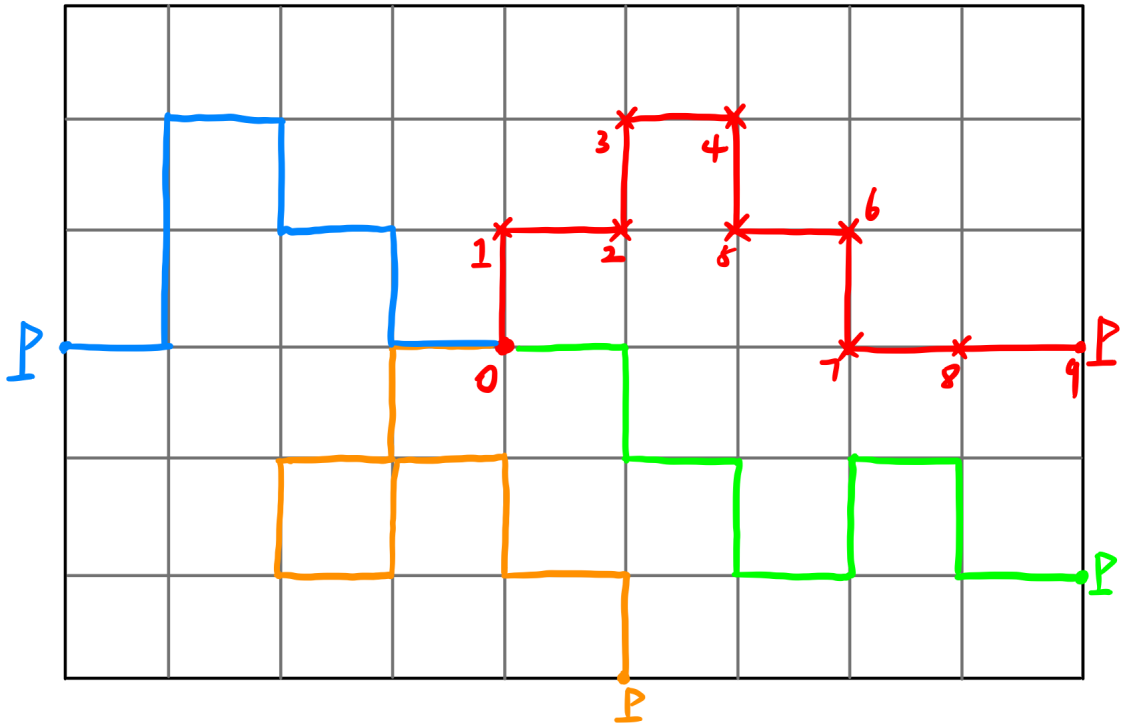
- $$\begin{aligned} \nabla^2 u &= 0 \quad \text{on} \quad G, \\ u &= f(x) \quad \text{on} \quad \partial G. \end{aligned}$$

- Discrete form with centered finite difference approximation,

$$u_{i,j} = \frac{1}{4}(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}).$$

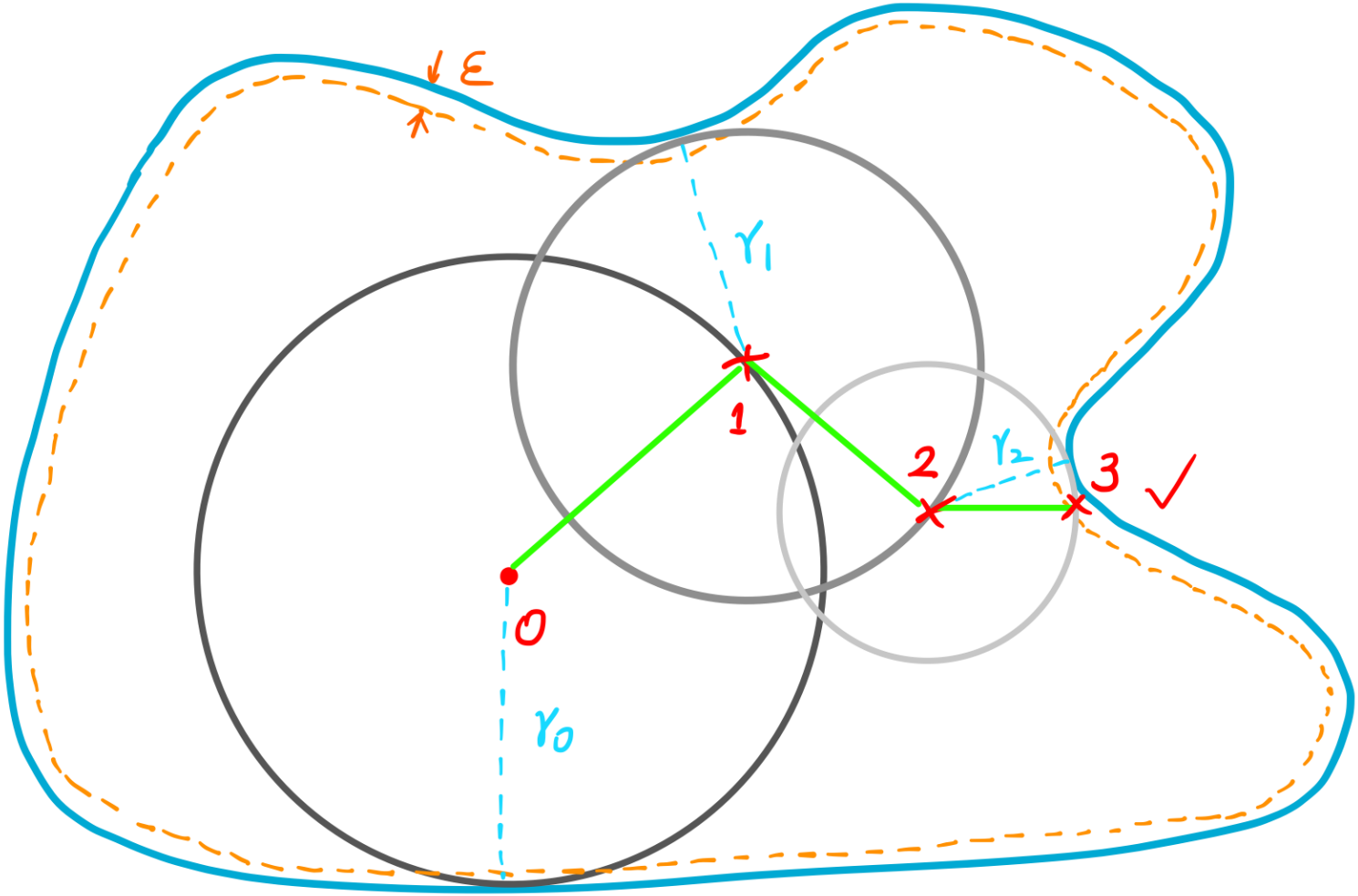


Simple Random Walk method



- For one random walk, we can get one estimate. Average over a large amount of estimates, we can get a precise value.
- The simple random walk is not very efficient, and the path doesn't really matter! We can improve it!
- Let grid spacing go to zero, random walk becomes Brownian motion.

Walk on Spheres method



- Much faster than the Simple Random Walk method.

Characteristics of Monte Carlo methods

- *Independence of points*: **The points to be evaluated are totally independent**. This makes the Monte Carlo methods **very suitable and efficient for evaluating values at certain points**.
- *Boundary & Dimension*: It's easier for the Monte Carlo methods to **handle complex boundaries** and to be **extended to higher dimensions**.
- *Parallel Computing*: Not only different points, but also different estimates for a given point are independent. This makes the Monte Carlo methods **naturally parallel**.

Parallelization

- The two straightforward ways to parallelize the program are,
  1. Parallelize the different estimates of one point, then average the results from different processes.
  2. Parallelize the set of points to be evaluated.
- For the first way,
  1. Allocate the estimates you want to get for every point to all available cores;
  2. Initialize the random number generator of different processes with different seeds, with *numpy.random.RandomState(seed)*.
  3. Wait for all the processes to finish, then collect and average the data.
- *Python* package *multiprocessing*.

Square Boundary

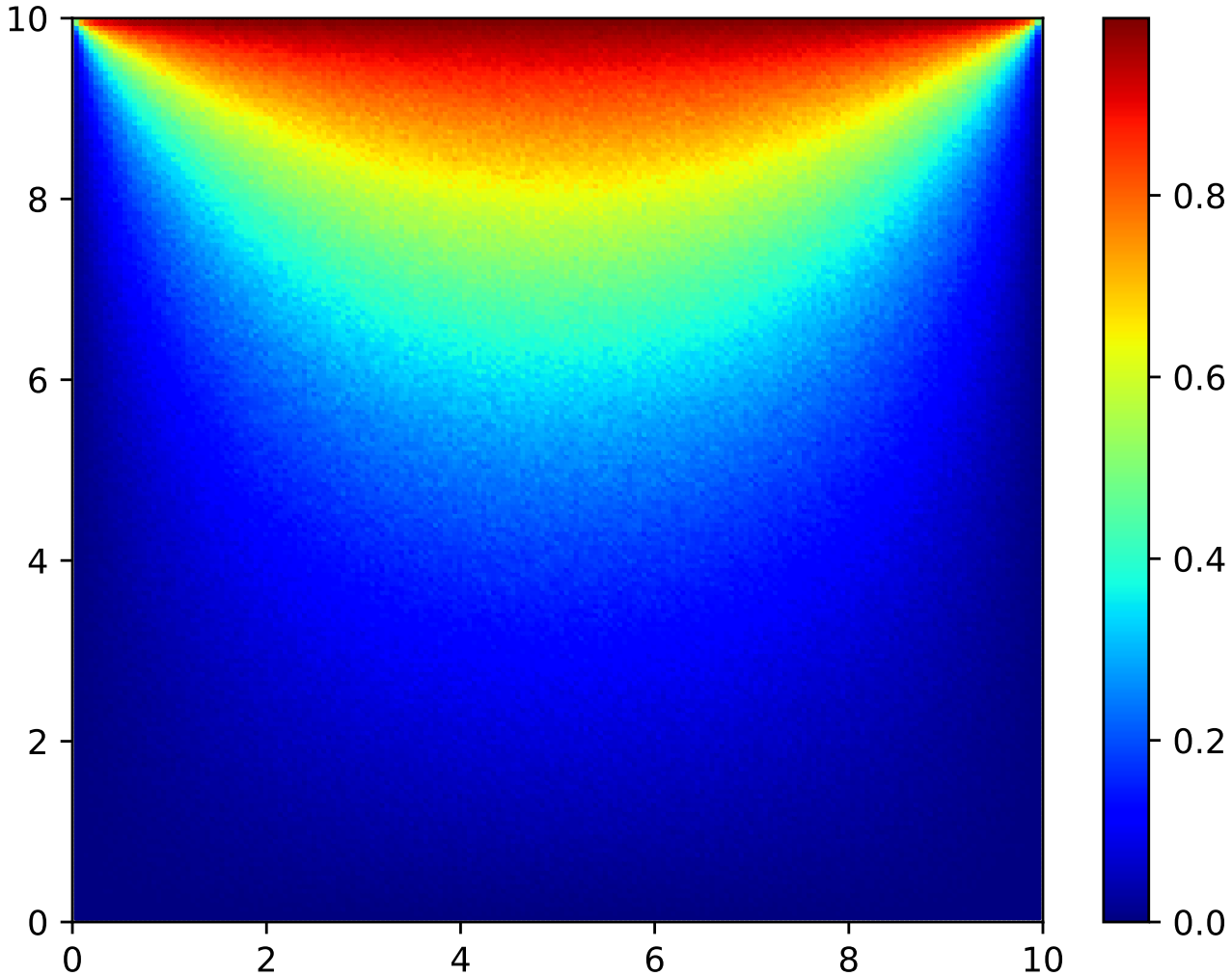


Figure: WoS method on 2D Square Boundary $(1, 0, 0, 0)$, 200×200 points, $2,000$ estimates for each point.

Circle Boundary

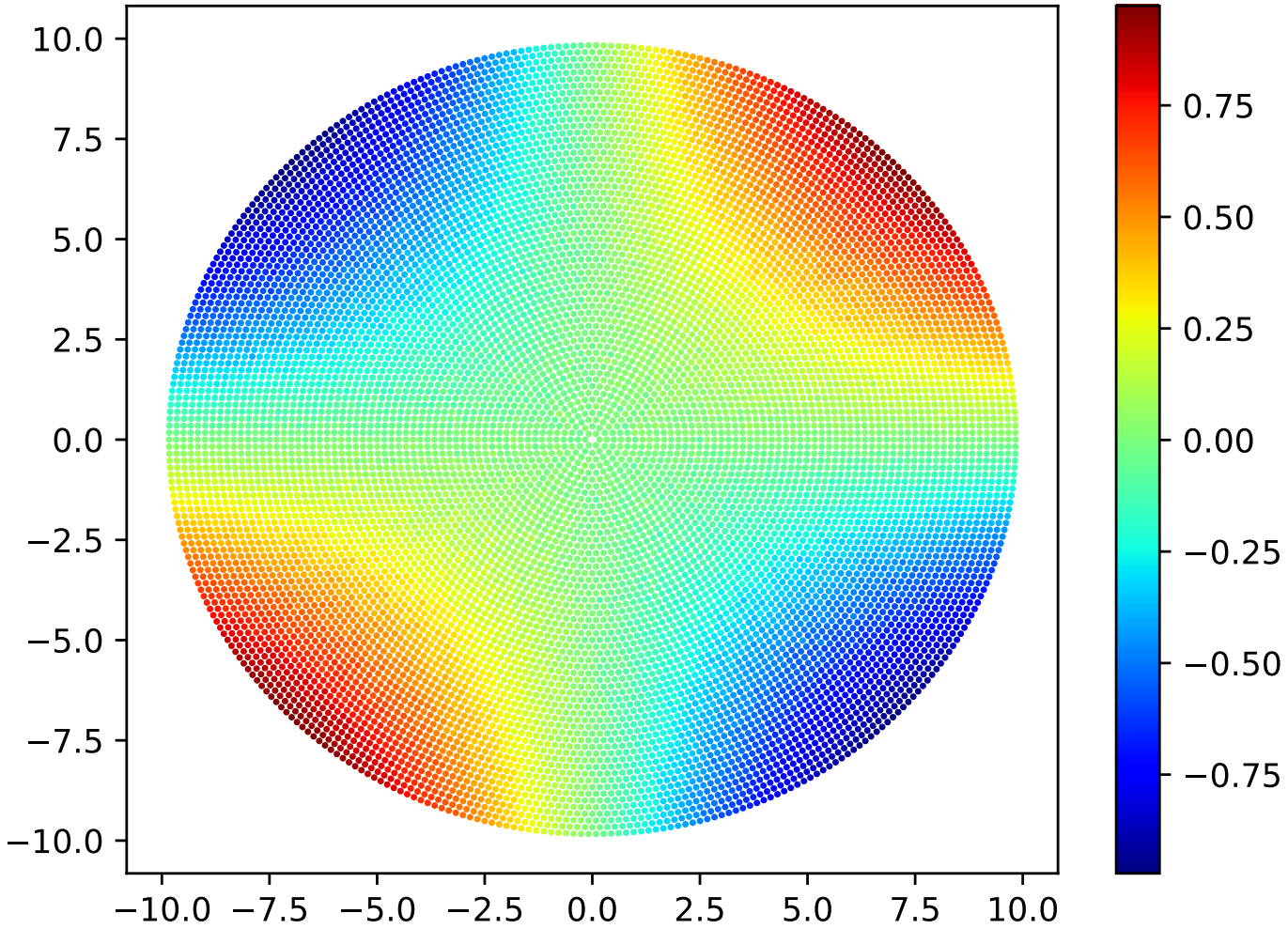


Figure: WoS method on 2D Circle Boundary ($\sin 2\theta$), $10,620$ points, $1,000$ estimates for each point.

Analysis of WoS method - Running time vs. ϵ

- $t = -k \log \epsilon + t_0$

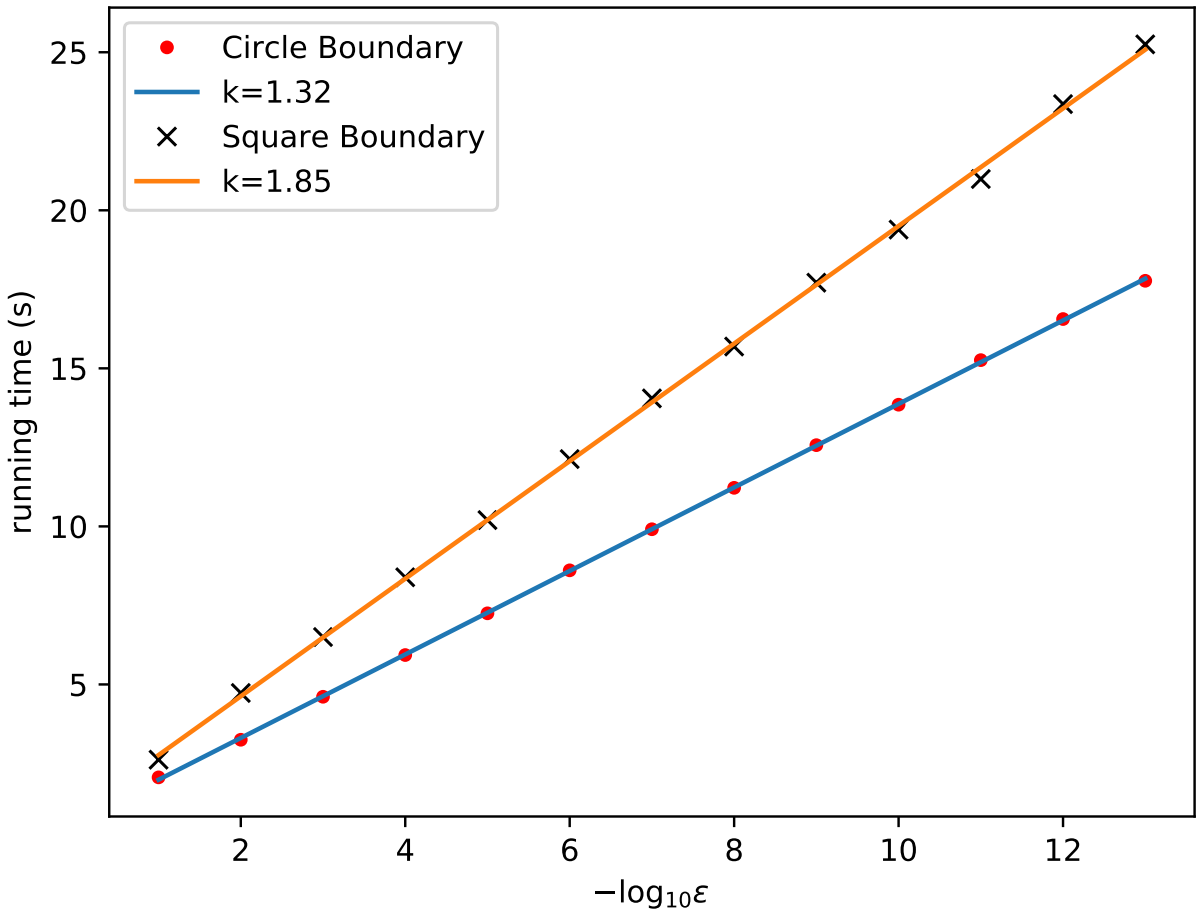


Figure: The running time - ϵ relation on both square and circle boundaries.

Analysis of WoS method - Convergence

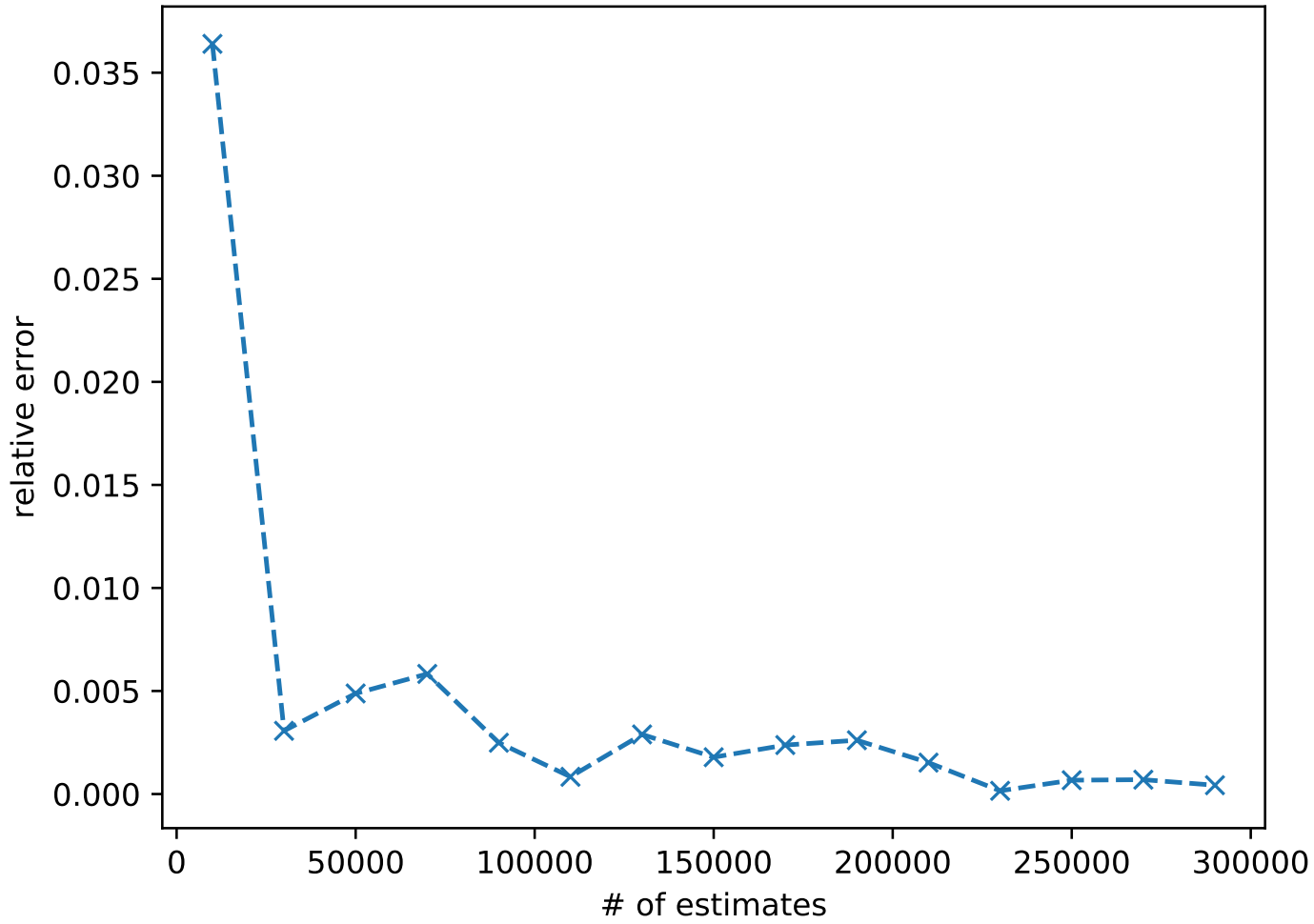


Figure: The convergence of the WoS method at the center point of the square boundary.

Future Work

- *Green's Function First Passage*:

$$p(x_0, x) = \frac{\partial G(x_0, x)}{\partial n}$$

  If we know the Green's Function for a domain, we can directly simulate the transition from the starting point to the boundary. Then we can get all the estimates directly.

- *Parallelization on GPU*:
  The Monte Carlo methods here are naturally parallel, so they may be accelarated a lot with GPU computing.

- *How things work for other PDEs*:
  e.g. Diffusion Equation etc.

Thank you! Questions?