

Merging Monte Carlo Methods with Machine Learning

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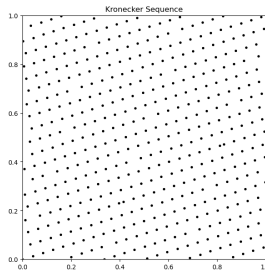
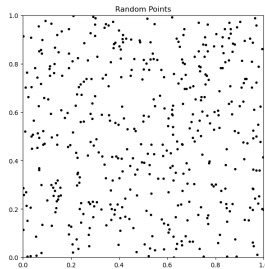
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Applied Mathematics

What are (quasi-)Monte Carlo methods?

Monte Carlo (MC) algorithms rely on **random sampling**.

Quasi-Monte Carlo (QMC) algorithms rely on **uniform sampling**. These sampling schemes are referred to as **low-discrepancy** point sets and sequences.



Discrepancy Theory

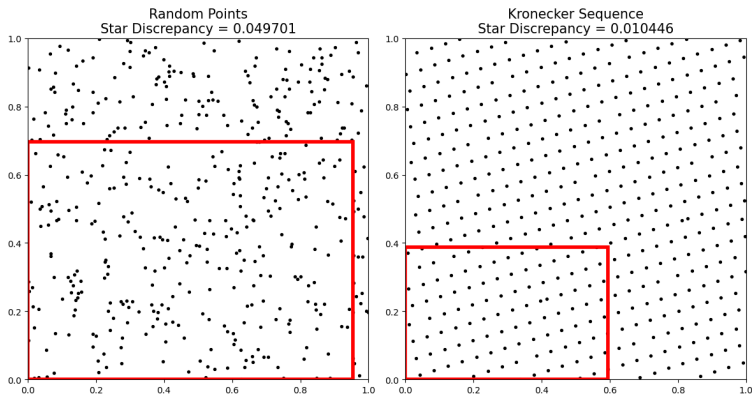
How can we quantify uniform distribution?

Let $\{\mathbf{X}_i\}_{i=1}^N$ be a point set contained in $[0, 1)^d$. The **(star) discrepancy** of $\{\mathbf{X}_i\}_{i=1}^N$, denoted $D^*(\{\mathbf{X}_i\}_{i=1}^N)$ is defined as,

$$D^*(\{\mathbf{X}_i\}_{i=1}^N) := \sup_{\mathbf{b} \in [0,1)^d} \left| \frac{\#([\mathbf{0}, \mathbf{b}) \cap \{\mathbf{X}_i\}_{i=1}^N)}{N} - |[\mathbf{0}, \mathbf{b})| \right|$$

- The star discrepancy is a discrete problem! We check N^d boxes.

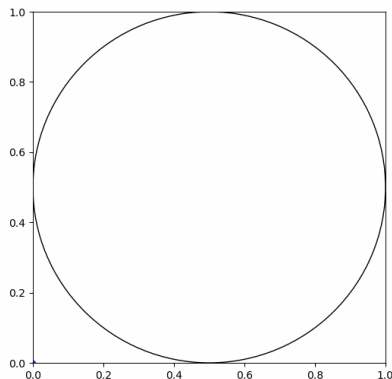
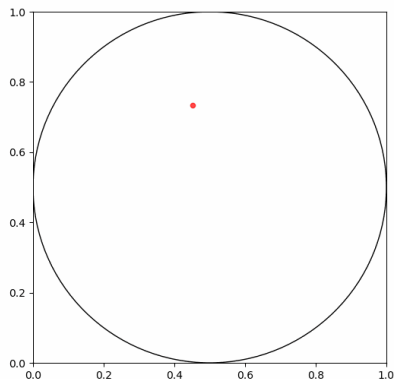
Discrepancy Theory - An example



Often intractable to compute in practise. Even in dimension as small as 3 depending on the number of points N .

Example: Approximating π

Monte Carlo vs. quasi-Monte Carlo

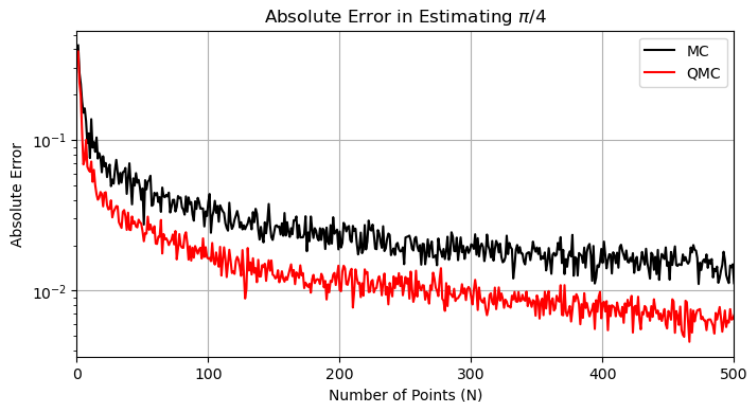


$$\frac{\#(\text{inside circle})}{\text{total points}} \rightarrow \frac{\pi}{4} \approx 0.785\dots$$

Example: Approximating π

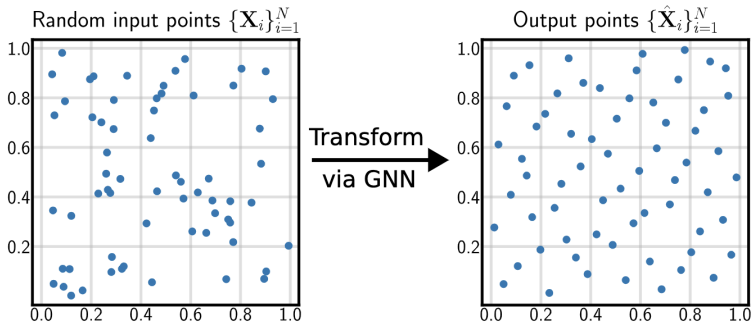
Monte Carlo vs. quasi-Monte Carlo

Plotting the error $\Rightarrow$ QMC gives smaller errors than MC



My recent work: Message-Passing Monte Carlo (MPMC)

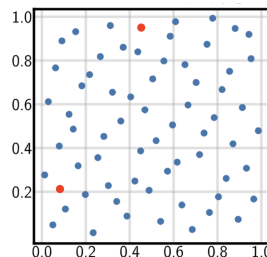
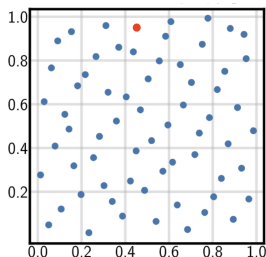
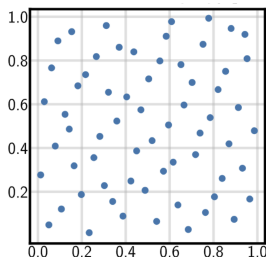
Published in PNAS, "Message-Passing Monte Carlo: Generating low-discrepancy point sets via graph neural networks", presents the **first machine learning approach** to construct low-discrepancy point sets using **graph neural networks**.



Available Projects for Collaboration - Project 1

Extending MPMC from fixed point sets to sequences

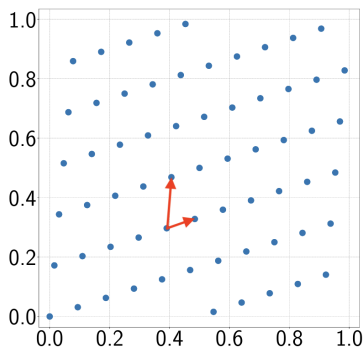
- Currently restricted to fixed N , i.e., to obtain an $N + 1$ set, one has to train again from scratch
- Most important open problem with MPMC
- Work already started by a Masters student at IIT



Available Projects for Collaboration - Project 2

Generating new lattice constructions with MPMC

- Lattices are an important class of QMC point set
- Can we optimize the generating vector to maximize uniformity? What about in higher dimensions?



Requirements for Collaboration

Essential:

- Demonstrable experience with PyTorch constructing machine learning models

Desirable:

- Experience working with graph neural networks
- Interest in Monte Carlo methods

Please approach me to chat afterwards, or email nkirk@iit.edu.

Thank you for listening!