Speedier Simulations with Quasi-Monte Carlo Methods

Final Presentation

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Overview

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Purpose of Quasi-Monte Carlo

Many problems can be written in the form of a multidimensional integral taken over the d-dimensional unit cube, which can be approximated by point evaluations:

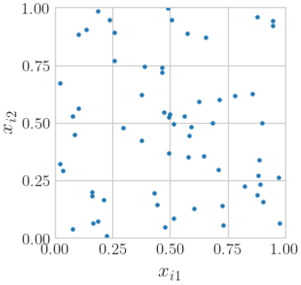
$$\int_{[0,1]^d} f(\mathbf{x})\, d\mathbf{x} \approx \frac{1}{n} \sum_{i=1}^{n} f(\mathbf{x}_i) \tag{1}$$

Quasi-Monte Carlo (QMC) methods use point sets $P_n = \{\mathbf{x}_i\}_{i=1}^{n} \subset [0,1]^d$ with ***low discrepancy***, while traditional Monte Carlo methods use IID (independent and identically distributed) points.

Low Discrepancy

Discrepancy = a measure of the difference between the empirical distribution of a set of points and the uniform distribution [5].

- In other words, how "evenly" a set of points fills the domain.
- Lower discrepancy = faster convergence and lower-variance estimates
- **Sobol'** points = a type of LD sequence



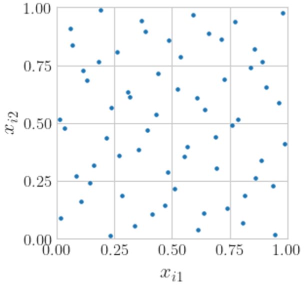


Figure 1: Left: IID, vs. right: low discrepancy (Sobol')

Overview

Kernel Density Estimation

Definition

Kernel Density Estimation is a non-parametric method for estimating probability distributions using kernels as weights

$$\hat{\rho}_h(y) = \frac{1}{n}\sum_{i=1}^{n} k_h(y - f(\boldsymbol{x}_i)) = \frac{1}{n}\sum_{i=1}^{n} \frac{1}{h} k\left(\frac{y - f(\boldsymbol{x}_i)}{h}\right)$$

KDE's rely on the **placement** and **distribution** of the data points. Thus, using low discrepancy (LD) sequences allows for density estimates with **reduced sampling bias** and **variance**, especially in higher dimensions [5].

Bandwidth Parameter

Bandwidth, denoted h, determines the amount of smoothing applied when estimating $\hat{\rho}(y)$ [6].

- Smaller h = less smoothing; larger h more smoothing.

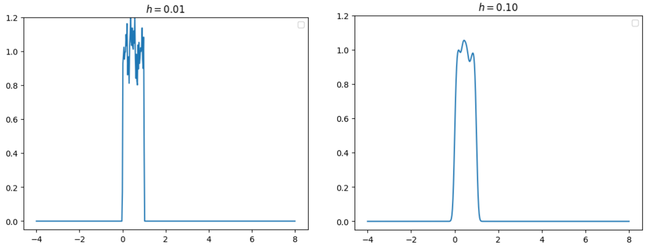


Figure 2: KDE for standard uniform distribution with smaller bandwidth (left) vs. larger bandwidth (right).

Objective of Error Analysis

- Study the effects of various factors on the accuracy of kernel density estimators.
- Factors/parameters include:
  - IID vs. Sobol' (LD) points
  - K = kernel function
  - n = sample size
  - h = bandwidth
  - d = dimension
  - $f(X)$ = function that transforms a set of IID or LD points X into a random variable with a known distribution

Parameters and Other Factors

- **Kernels**: Epanechnikov and Gaussian [5]
- **Bandwidths**: 100 different values in the range (0, 1], defined on a power scale: $\{h_i\} = 2^{\{a_i\}}$ where $\{a_i\}$ is the set of 100 evenly-spaced points between -10 and 0, inclusive.
- **Sample sizes**: $\{2^{10}, 2^{11}, 2^{12}, 2^{13}, 2^{14}\}$
- **Distributions**:
  - **1-dimensional**: standard Uniform, standard Gaussian, exponential (with $\lambda = 1$), Laplace (with $\mu = 0$ and $b = 1$), and chi-squared (with $\mathrm{df} = 1$).
  - **Multi-dimensional**: triangular (sum of 2 standard uniforms), sum of 3 and 5 standard Gaussians, and chi-squared with $\mathrm{df} = 3$ and $\mathrm{df} = 5$ (i.e., sum of 3 and 5 squared Gaussians).

Definition of RMSE

Definition

The **root mean square error (RMSE)** measures the average difference between the expected values and predicted values of a probability density function:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{\rho}(y_i) - \rho(y_i))^2} \tag{2}$$

Finding Minimum RMSE and Optimal Bandwidth

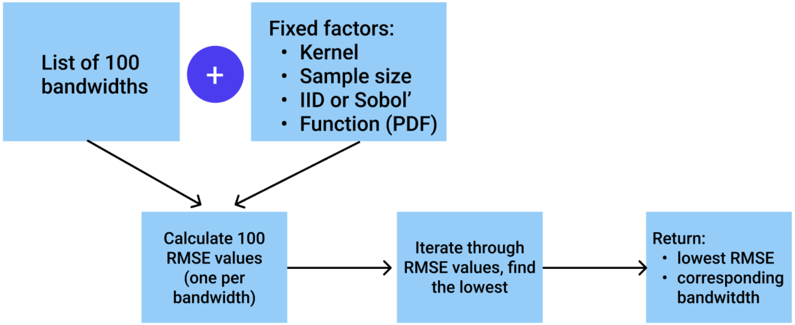

List of 100 bandwidths
+
Fixed factors:
• Kernel
• Sample size
• IID or Sobol'
• Function (PDF)
Calculate 100 RMSE values (one per bandwidth)
Iterate through RMSE values, find the lowest
Return:
• lowest RMSE
• corresponding bandwitdth

Figure 3: Flowchart to find optimal bandwidth using RMSE calculations. This procedure is performed for each set of factors and parameters that we test.

Results: RMSE vs. n

- We plotted four regression models of the form

$$-\log_{10}(RMSE) = b_0 \cdot \log_{10}(n) + \sum_{j=1}^{N} b_j \cdot x_j + \varepsilon_j, \tag{3}$$

where b_0 is the slope of $-\log_{10}(RMSE)$ vs. $\log_{10}(n)$, and x_j are indicator variables to separate the N different distributions we tested.

Table 1: Coefficients b_0 for linear regression models of log-scaled RMSE vs. log-scaled sample size.

	1-dim	**Multi-dim**
IID	0.8379	0.8811
Sobol'	1.0750	0.9465

Results: RMSE vs. n (con't)

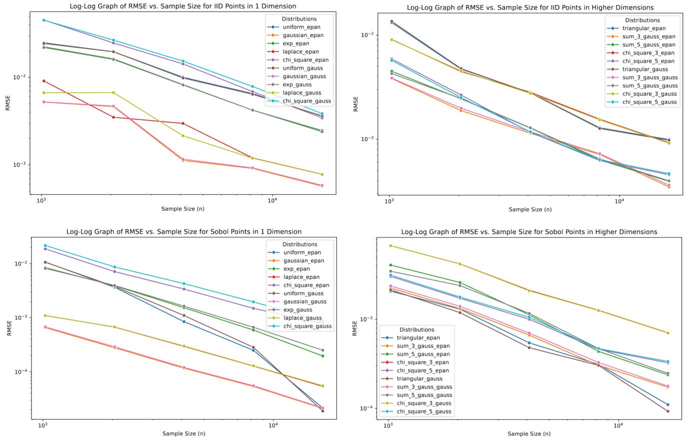


Figure 4: Log-log graphs of RMSE vs. sample size (n) based on Equation (3). For IID points, slope in 1 dim. is 0.8379 (top left) and in higher dims. is 0.8811 (top right). For Sobol' points, slope in 1 dim. is 1.0750 (bottom left) and in higher dims. is 0.9465 (bottom right).

Results: Optimal Bandwidth vs. n

- We plotted four regression models of the form

$$-\log_{10}(h) = b_0 \cdot \log_{10}(n) + \sum_{j=1}^{N} b_j \cdot x_j + \varepsilon_j, \tag{4}$$

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Table 2: Coefficients b_0 for linear regression models of log-scaled optimal bandwidth vs. log-scaled sample size.

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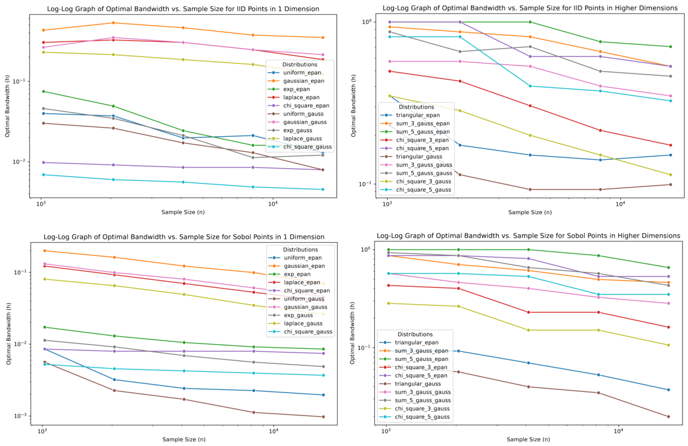

Figure 5: Log-log graphs of optimal h vs. sample size (n) based on Eq. (4). For IID points, slope in 1 dim. is 0.2889 (top left) and in higher dims. is 0.2747 (top right). For Sobol' points, slope in 1 dim. is 0.3374 (bottom left) and in higher dims. is 0.2818 (bottom right).

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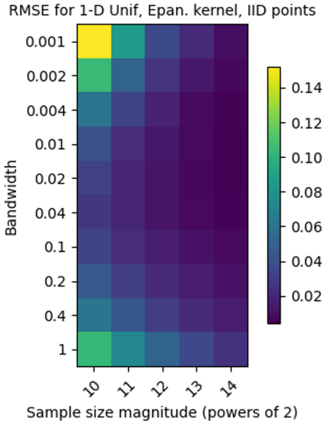

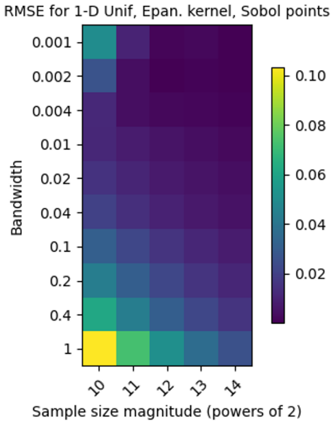

Figure 6: RMSE values (shaded) for different sample sizes and bandwidths when estimating the 1-dimensional standard uniform distribution using the Epanechnikov kernel.

Thoughts and Future Work

- Advantages of using Sobol' (LD) points vs. IID points
- Tailoring bandwidth specifically based on distribution & sample size
- *Future work*: testing different distributions, higher dimensions, different sets of bandwidths; theoretical work to illustrate relationships

Conditional Density Estimation

Let $Y = f(X_1, ..., X_d)$ such as

$$Y = X_1^2(X_2 + 3X_3)$$

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Let $f(X_1, \ldots, X_d \,|\, \mathcal{G}_{-k}) =: g(X_k; \mathcal{G}_{-k})$

$$F(y \,|\, \mathcal{G}_{-k}) = P(Y \leq y \,|\, \mathcal{G}_{-k}) = P(X_k \leq g^{-1}(y) \,|\, \mathcal{G}_{-k}) = F_k(g^{-1}(y))$$

This gives a conditional density $\rho(y \,|\, \mathcal{G}_{-k}) = \frac{d}{dy} F_k(g^{-1}(y))$

With QMC

Theorem

Suppose we have $\rho(y|\mathcal{G}_{-k})$ that satisfies certain technical assumptions. Then

$$\mathrm{E}[\rho(y \mid \mathcal{G}_{-k})]_{\mathcal{G}_{-k}} = \rho(y) \tag{5}$$

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Under slight modification, we can use QMC to help approximate this expectation. The dimension is one less than the dimension of a standard KDE since we only need to realize $d - 1$ variables!

Experimental Methodology

The usual measure of error is the MISE $= \int_a^b \mathrm{E}[(\rho(y) - \hat{\rho}_n(y))^2]\, dy$

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$$\widehat{\text{MISE}} = \frac{b-a}{n_e} \sum_{i=1}^{n_e} \text{var}[\hat{\rho}_n(y_i)]_{n_r}$$

Thus, as we vary n, we can get $\widehat{\text{MISE}}(n)$ and fit it to a power law

$$\widehat{\text{MISE}}(n) = Kn^{-\nu}$$

Example 1: Weighted Sum Uniform

$Y = X_1 + X_2 + X_3$ for $X_j \sim \mathcal{U}([0, 2^{j-1}])$

$$\rho(y \mid \mathcal{G}_{-k}) = \begin{cases} 2^{1-k} & y - \sum_{i \neq k} X_i \in [0, 2^{k-1}] \\ 0 & \text{else} \end{cases}$$

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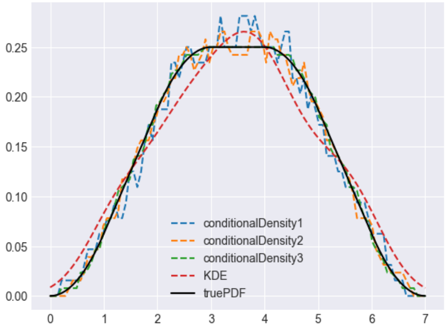

Figure 7: Plotting the conditional densities with Sobol' for $n = 32$ with a KDE and true PDF

Error graph

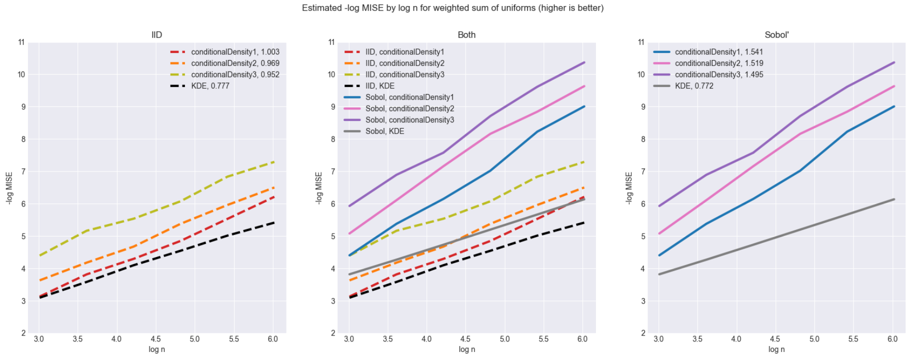

Figure 8: -log, log plot. The slopes of IID hover around 1, KDE around 0.8, and Sobol' around 1.5. Best conditional density is conditionalDensity3.

Example 2: Cantilevered Beam

$Y = \frac{\kappa}{X_1}\sqrt{\frac{X_2^2}{256} + \frac{X_3^2}{16}}$ for $X \sim \mathcal{N}(\mu_j, \sigma_j^2)$ with
$\kappa = 5 \cdot 10^5, \mu = (2.9 \cdot 10^7, 500, 1000)$ and $\sigma = (1.45 \cdot 10^6, 100, 100)$
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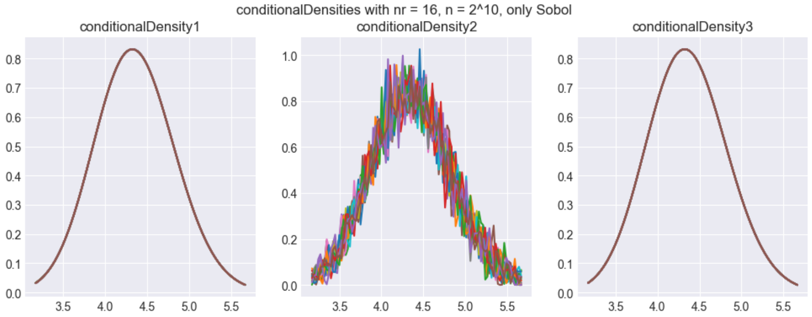

Figure 9: Plotting the conditional densities with Sobol' for $n = 1024$ over $nr = 16$ repetitions

Error graph

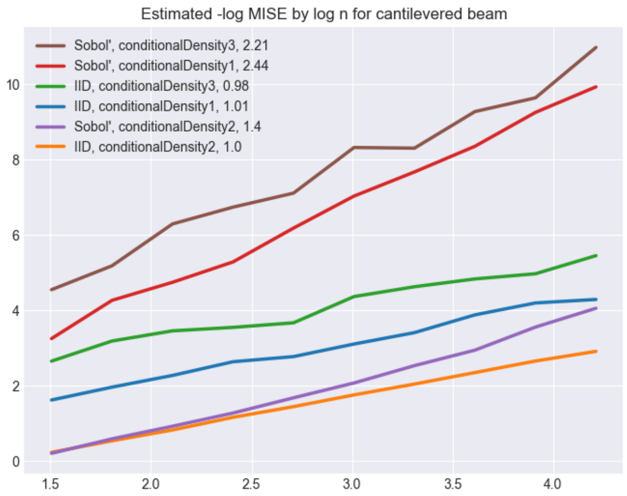

Figure 10: -log, log plot. Slope of IID hover around 1. conditionalDensities vary a lot. Sobol' better than IID

Thoughts

- Conditional density estimation, when applicable, is much less cumbersome and much better than KDE
- Most of these are toy examples; certain real examples (like options pricing) require much more care and attention
- The effect is most noticeable when certain variables contribute to a large portion of the variance
- Interesting work will continue in applying conditional densities estimates to different classes of problems

Overview

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- The **Kernel Trick** is a powerful technique for modeling non-linear relationships using linear learning algorithms by implicitly mapping data into a higher-dimensional feature space using a kernel function.
- Why are Kernels Defined on Discrete input Spaces Useful?
  - Various real-world applications: bio-informatics, community detection, manifold learning for deep generative modeling, etc... [3]

Applying Kernels to Combinatorial Objects

- **Kernel Function**: For discrete objects, like graphs, we define a *graph kernel* (or kernel function) as $K : \mathcal{X} x \mathcal{X} \rightarrow \mathbb{R}$ which returns a real number representing the similarity measure between these structures

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- **Gram (Kernel) Matrix**: Kernel evaluations are stored in a Gram Matrix $\mathbf{K} \in \mathbb{R}^{NxN}$ whose entries enumerate the pairwise kernel evaluations $\mathbf{K} := [K(x_i, x_j)]_{i,j=1}^{N}$
  - Entries of this matrix represent similarities between each pair of data points

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    - **Randomised Function**: $\phi : \mathbb{R}^d \to \mathbb{R}^s$ maps the original data points into a lower dimensional space
    - **Low-Dimensional Feature Vector**: whose dot product approximates the kernel function: $\mathbf{K}_{ij} = \mathbb{E}[\phi(x_i)^\intercal \phi(x_j)]$ meaning the dot product of the transformed vectors is an unbiased estimator of the kernel function

Graph Random Features

- A recently viable **Graph Random Features** (GRFs) mechanism employs an ensemble of random walkers that deposit a "load" at every vertex they pass, depending on
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- **Key Limitation**: Only addresses a niche family of graph kernels

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- The key contribution to g-GRFs is the **Modulation Function**, f, that controls the weight of the load deposited by random walkers as they traverse the graph based on the length of the walk
- By parameterizing this modulation function on a **Neural Network**, the algorithm provides an efficient, unbiased approximation of the desired graph kernel

Quasi-Monte Carlo Graph Random Features

Can we improve the accuracy and efficiency of g-GRFs?

- **Quasi-Monte Carlo Graph Random Features** (q-GRFs) introduces correlated ensembles, or antithetic walkers, to correlate the lengths of random walks with some stopping criterion [4]

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  - In the IID implementation (g-GRFs) two termination random variables (TRVs) are sampled independently from from a uniform distribution $t_{1,2}$ $Unif(0,1)$. Each walker terminates if their respective TRV $t_{1,2} < p$
  - **Antithetic Walkers**: A pair of walkers are antithetic if their TRVs are marginally distributed as $t_{1,2} \sim \mathcal{U}(0,1)$ but are offset by $\frac{1}{2}$,

$$t_2 = \text{mod}_1\left(t_1 + \frac{1}{2}\right), \tag{6}$$

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  - Diversifying the lengths of random walks prevents clustering; therefore, Choromanski, Reid, and Weller assert that antithetic walkers (q-GRFs) yield lower variance estimators of the 2-regularised Laplacian kernel

Our Investigation

- **Motivating Question**: Can we identify an alternative kernel function or graph type where q-GRFs achieve a lower variance estimator like the previously introduced 2-Regularised Laplacian kernel?
    - Diffusion (or Heat), Matérn, Inverse Cosine Kernels
    - Erdős-Rényi and Barabási-Albert random graph models, Binary Trees, and Ladder graphs

Diffusion (or Heat) Kernel

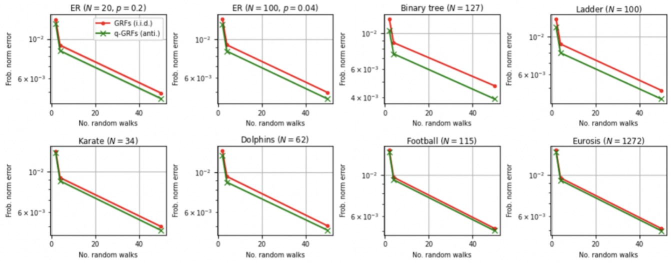
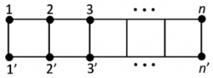


Figure 11: Relative Frobenius norm error of estimators of the diffusion (or heat) kernel with $t = 0.5$ using g-GRFs (red circles) and q-GRFs (green crosses). **Lower is better**. N gives the number of nodes and p is the edge-generation probability for the Erdös-Rényi graphs. One standard deviation is shaded.

Ladder Graphs



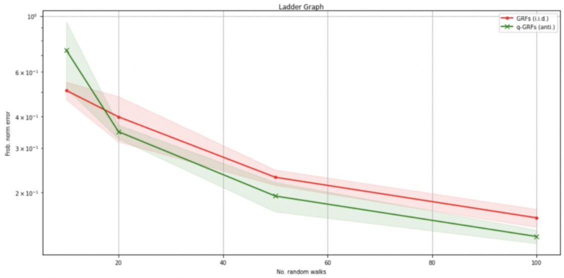


Figure 12: LEFT: Standard ladder graph. RIGHT: Ladder graph with number of random walks set to (10, 20, 50, 100) and number of rungs set to 9. Q-GRFs yield lower variance estimators of the diffusion kernel than general g-GRFs.

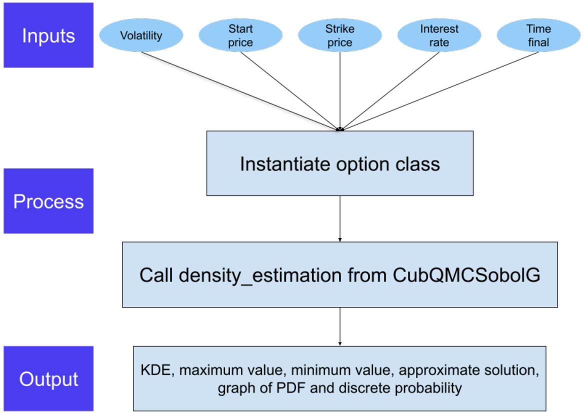
Results and Future Work

- Despite the inherent randomness in the antithetic procedure, there is strong evidence to suggest that q-GRFs have the potential to yield lower variance estimators of the diffusion kernel – though further experimentation and theoretical work is necessary to make final conjectures
- We assert that the **number of rungs** on a ladder graph impacts q-GRFs ability to achieve a lower variance estimator of the diffusion kernel
- Further theoretical results investigating these phenomena are forthcoming

QMC Application for Finance Options

- Use QMC to estimate the PDF of the payoff of an option.
- QMC allows faster computation than regular MC.
- QMCPy allows someone to compute such estimations.

QMC Application for Finance Options



Inputs
Volatility
Start price
Strike price
Interest rate
Time final
Process
Instantiate option class
Call density_estimation from CubQMCSobolG
Output
KDE, maximum value, minimum value, approximate solution, graph of PDF and discrete probability

Figure 13: Flowchart of using an option class.

European Density Estimation

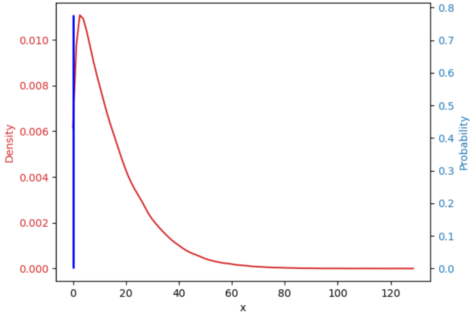


Figure 14: PDF of the payoff for a European option with starting price of \$100 and strike price of \$120, with interest rate of %0.5, and volatility of 0.2.

Pull Request

- Finish code that was in development by a graduate student.
- Review code before merging into the main development branch.
- Satisfy requested changes to the code before finally merging.
- Begin merging said code into the main development.

Refactoring

- **Issue:** Code among the option classes have the same code.
- **Solution:** Refactored all option classes to remove duplicate code.

Refactoring

What does refactoring mean?

Definition

Refactor: a change made to the internal structure of software to make it easier to understand and cheaper to modify without changing its observable behavior.[1]

Refactoring

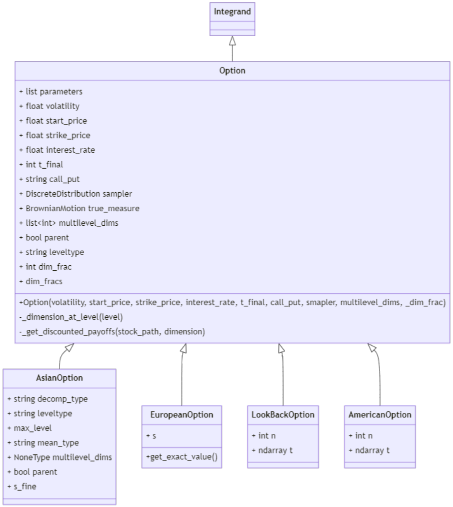


Figure 15: UML Class diagram of all option classes.

Conclusion

Important things learned and encountered when developing robust scientific software:

- Use software engineering principles.
- Structure your code and write everything to be clear.
- Use the documentation of the language and libraries to help build the software.

Overview

Conclusion and Final Thoughts

- Low discrepancy points can provide much lower error than IID uniform points in a variety of situations:
  - Density estimations (using kernels & conditioning)
  - Analyzing combinatoral objects
  - Modeling financial options
- Theoretical analysis, further applications, and robust implementation are key to maximizing the potential of low discrepancy points

Thank you!

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Appendix A: Links

- KDE Error Analysis: Final report and Python notebook
- https://qmcpy.org/
- https://github.com/QMCSoftware/QMCSoftware
- Conditional QMC: Report and Python notebooks 1 and 2
- QMC with combinatorial objects: Final report and Python notebook

Appendix B: Epanechnikov vs. Gaussian Kernel

Definition

The **Gaussian** kernel is defined with the weighting function

$$w(y,h) = \frac{1}{2\pi h} e^{-\frac{y^2}{2h^2}}, \qquad -\infty < y < \infty \tag{7}$$

Definition

The **Epanechnikov** kernel is defined with the weighting function

$$w(y,h) = \begin{cases} \frac{3}{4h}(1 - \frac{y^2}{5h^2})/\sqrt{5} & \text{for } |y| < \sqrt{h}, \\ 0 & \text{otherwise.} \end{cases} \tag{8}$$

- The above weighting functions, $w(y,h)$, are all of the form $w(y,h) = \frac{1}{h}K(\frac{y}{h})$, where K is the *kernel* function [6].

Appendix B: Epanechnikov vs. Gaussian Kernel (con't)

The Epanechnikov kernel has an efficiency of 100%, while the Gaussian kernel has an efficiency of 95.12%, where the *efficiency* of a kernel is defined as:

$$\text{Efficiency}(K) = \left(\frac{RMSE_{opt}(\hat{\rho}) \text{ using } K_{EP}}{RMSE_{opt}(\hat{\rho}) \text{ using } K} \right)^{\frac{5}{4}} \tag{9}$$

This means that the RMSE obtained using an Epanechnikov kernel with $n \approx 95$ is approximately equal to the RMSE obtained using a Gaussian kernel with $n = 100$ [5].

Appendix B: Epanechnikov vs. Gaussian Kernel (con't)

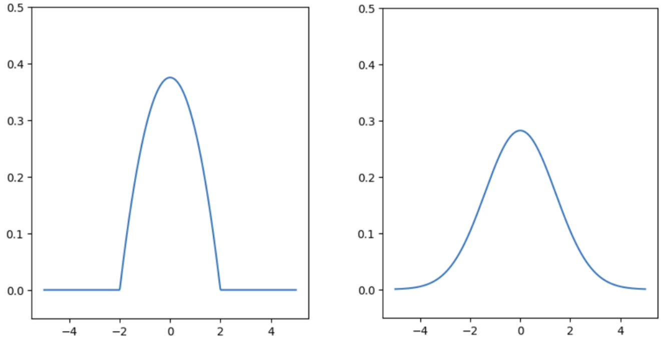

Figure 16: Shape of the Epanechnikov (left) vs. the Gaussian kernel (right). The kernel determines the shape of the weighting function.