Faster Monte Carlo via Low Discrepancy Sampling

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Thank you for your invitation and hospitality,
Slides at speakerdeck.com/fjhickernell/argonne2023maytalk
Jupyter notebook with computations and figures here   Visit us at qmcpy.org

Argonne Seminar, revised Wednesday 24th May, 2023

Family of Physicists

- Fred S. Hickernell (father), PhD Physics, IEEE Fellow, Motorola researcher
- Robert K. Hickernell (brother), PhD Physics, NIST Division Director
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- Myself, BA mathematics and physics who became an applied mathematician

Message

Problems in Bayesian inference, uncertainty quantification, quantitative finance, (high energy) physics[1], etc. require numerically evaluating

$$\underbrace{\mathbb{E}[f(\boldsymbol{X})]}_{\text{expectation}} = \underbrace{\int_{\Omega} f(\boldsymbol{x})\, \varrho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x},}_{\text{integral}} \qquad \boldsymbol{X} \sim \varrho$$

Other more complicated problems include computing quantiles or marginal distributions.

[1] M. R. Blaszkiewicz (Feb. 2022). "Methods to optimize rare-event Monte Carlo reliability simulations for Large Hadron Collider Protection Systems". MA thesis. University of Amsterdam. URL: https://cds.cern.ch/record/2808520; A. Courtoy, J. Huston, et al. (2023). "Parton distributions need representative sampling". In: *Phys. Rev. D* 107.034008. URL: https://journals.aps.org/prd/pdf/10.1103/PhysRevD.107.034008; D. Everett, W. Ke, et al. (May 2021). "Multisystem Bayesian constraints on the transport coefficients of QCD matter". In: *Phys. Rev. C* 103.5. DOI: 10.1103/physrevc.103.054904; D. Liyanage, Y. Ji, et al. (Mar. 2022). "Efficient emulation of relativistic heavy ion collisions with transfer learning". In: *Phys. Rev. C* 105.3. DOI: 10.1103/physrevc.105.034910.

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There is value in

- low discrepancy sampling, aka quasi-Monte Carlo methods
- data-driven error bounds
- flattening and reducing the effective dimension of the integrand
- quality quasi-Monte Carlo software like qmcpy[1]
- physicists and quasi-Monte Carlo theorists collaborating more

[1] S.-C. T. Choi, F. J. H., et al. (2023). *QMCPy: A quasi-Monte Carlo Python Library (versions 1–1.4)*. DOI: 10.5281/zenodo.3964489. URL: https://qmcsoftware.github.io/QMCSoftware/.

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Caveat: I know little about Markov Chain Monte Carlo (MCMC); limited success combining with quasi-Monte Carlo[2].

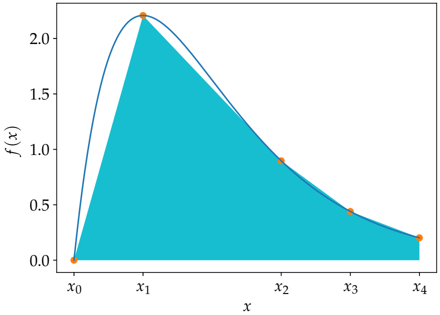
[2] S. Chen, J. Dick, and A. B. Owen (2011). "Consistency of Markov Chain Quasi-Monte Carlo on Continuous State Spaces". In: *Ann. Stat.* 9, pp. 673–701; Art B. Owen and Seth D. Tribble (2005). "A quasi-Monte Carlo Metropolis algorithm". In: *Proc. Natl. Acad. Sci.* 102, pp. 8844–8849.

Trapezoidal rule

Trio identity[3] — the error of approximating an expectation or integral expressed as the product of three quantities

$$\int_0^1 f(x)\,\mathrm{d}x - \sum_{i=0}^{n} w_i f(x_i) = 0.112 \qquad w_i = \frac{x_{i+1} - x_{i-1}}{2}$$

$$= \underbrace{\frac{\int_0^1 f(x)\,\mathrm{d}x - \sum_{i=0}^{n} w_i f(x_i)}{\frac{\max_i (x_{i+1}-x_i)^2}{8} \int_0^1 |f''(x)|\,\mathrm{d}x}}_{\substack{\text{misfortune} \\ 0.151}} \underbrace{\frac{\max_i (x_{i+1}-x_i)^2}{8}}_{\substack{\text{sampling deficit} \\ 0.020}} \underbrace{\int_0^1 |f''(x)|\,\mathrm{d}x}_{\substack{\text{roughness} \\ 37.3}}$$



[3] F. J. H. (2018). "The Trio Identity for Quasi-Monte Carlo Error Analysis". In: *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Stanford, USA, August 2016*. Ed. by P. Glynn and A. Owen. Springer Proceedings in Mathematics and Statistics. Springer-Verlag, Berlin, pp. 3–27. DOI: 10.1007/978-3-319-91436-7; A. Courtoy, J. Huston, et al. (2023). "Parton distributions need representative sampling". In: *Phys. Rev. D* 107.034008. URL: https://journals.aps.org/prd/pdf/10.1103/PhysRevD.107.034008; X. Meng (2018). "Statistical Paradises and Paradoxes in Big Data (I): Law of Lage Popluations, Big Data Paradox, and 2016 US Presidential Election". In: *Ann. Appl. Stat.* 12, pp. 685–726.

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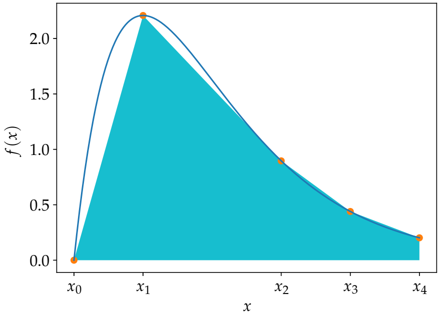

- Confounding is between -1 and 1 (Brass and Petras 2011, (7.15))
- Discrepancy depends upon sample only
- Variation depends on integrand only, semi-norm

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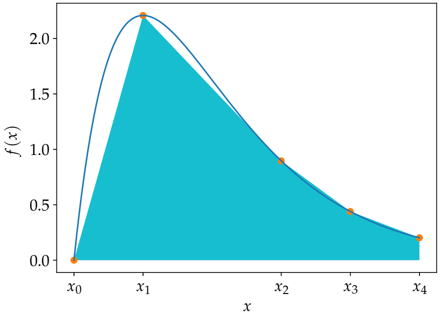

- Confounding is between -1 and 1 (Brass and Petras 2011, (7.15))
- Discrepancy reduced via clever or more sampling
- Variation value unknown, reduced via transformations

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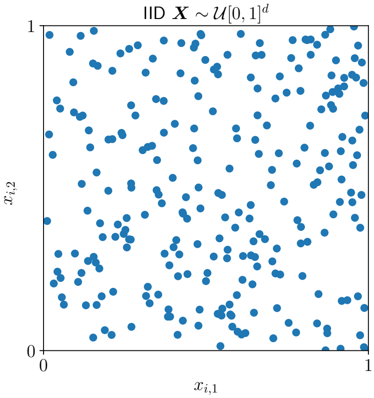
Independent and Identically Distributed (IID) Monte Carlo

$$\overbrace{\int_{\mathbb{R}^d} f(\boldsymbol{x})\, \varrho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}}^{\mathbb{E}[f(\boldsymbol{X})],\ \boldsymbol{X}\sim\varrho} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i) \qquad \boldsymbol{x}_i \overset{\text{IID}}{\sim} \varrho$$

$$= \underbrace{\frac{\int_{\mathbb{R}^d} f(x)\, \varrho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i)}{\frac{1}{\sqrt{n}}\ \mathrm{std}[f(\boldsymbol{X})]}}_{\text{confounding}} \ \underbrace{\frac{1}{\sqrt{n}}}_{\text{discrepancy}} \ \underbrace{\mathrm{std}(f(\boldsymbol{X}))}_{\text{variation}}$$

- $\mathrm{RMS}[\text{confounding}] = 1$, but confounding could be $\mathcal{O}(\sqrt{n})$
- Discrepancy depends on sample size only
- Variation reduced through transformations



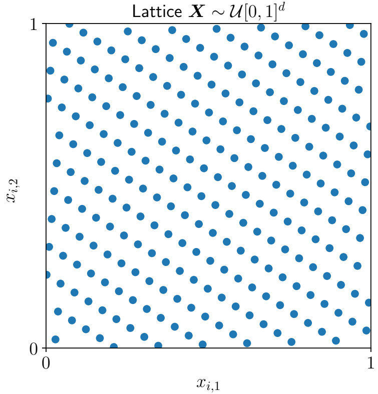
Low Discrepancy Sampling aka Quasi-Monte Carlo[4]

$$\overbrace{\int_{[0,1]^d} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}}^{\mathbb{E}[f(\boldsymbol{X})],\ \boldsymbol{X}\sim\mathcal{U}[0,1]^d} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i) = \mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{DSC}(\{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{VAR}(f)$$

$$\mathrm{VAR}^2(f) = \int_{[0,1]} \left[\frac{\partial f}{\partial x_1}(x_1, 0.5, \ldots, 0.5)\right]^2 \mathrm{d}x_1 + \cdots$$

$$+ \int_{[0,1]^2} \left[\frac{\partial^2 f}{\partial x_1 \partial x_2}(x_1, x_2, 0.5, \ldots, 0.5)\right]^2 \mathrm{d}x_1\, \mathrm{d}x_2 + \cdots$$

$$+ \int_{[0,1]^d} \left[\frac{\partial^d f}{\partial x_1 \cdots \partial x_d}(\boldsymbol{x})\right]^2 \mathrm{d}\boldsymbol{x}$$



VAR is a semi-norm, more smoothness than std, value generally unknown, reduced through transformations

[4] F. J. H. (1998). "A Generalized Discrepancy and Quadrature Error Bound". In: *Math. Comp.* 67, pp. 299–322. DOI: 10.1090/S0025-5718-98-00894-1.

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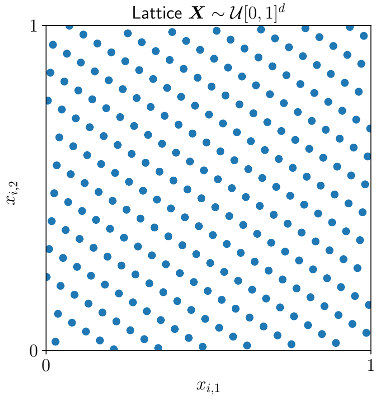
$$\mathrm{DSC}^2(\{\boldsymbol{x}_i\}_{i=1}^n) = \left(\frac{13}{12}\right)^2 - \frac{2}{n}\sum_{i=1}^{n}\prod_{j=1}^{d}\left(1 + 0.5\,|x_{ij} - 0.5| - 0.5(x_{ij} - 0.5)^2\right) + \frac{1}{n^2}\sum_{i,k=1}^{n}\left[1 + 0.5\,|x_{ij} - 0.5| + 0.5\,|x_{kj} - 0.5| - 0.5\,|x_{ij} - x_{kj}|\right]$$



$$\mathrm{DSC}(\{\boldsymbol{x}_i\}_{i=1}^n) = \mathcal{O}(n^{-1+\delta})$$

DSC is the norm of the error functional, value known with $\mathcal{O}(dn^2)$ operations

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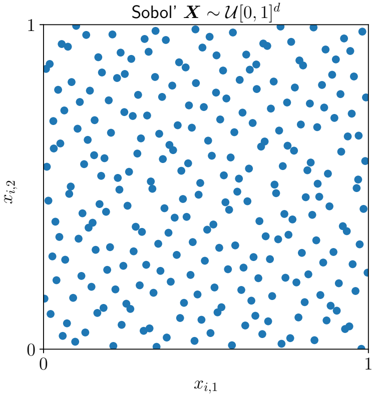

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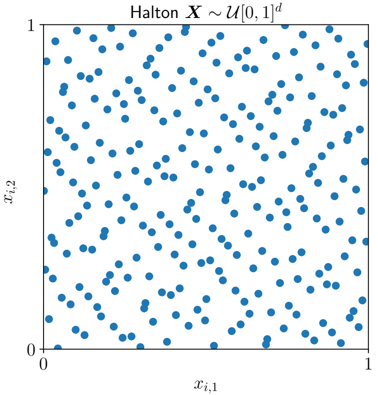

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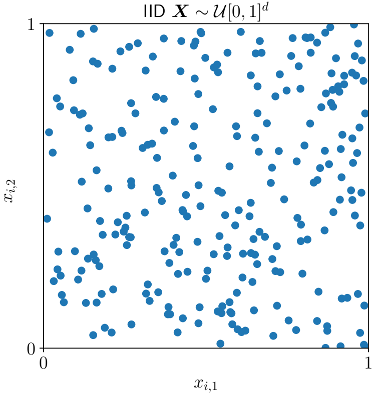

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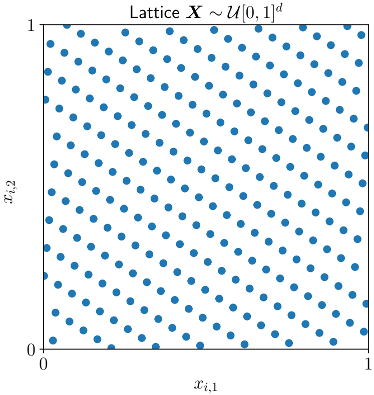

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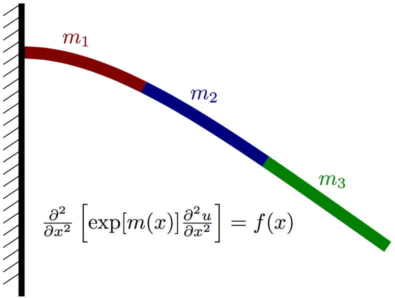
Uncertainty in a Cantilevered Beam[5]

$$u(x) = g(\mathbf{Z}, x) = \text{beam deflection}$$
$$= \text{solution of a differential equation boundary value problem}$$
$$\mathbf{Z} \sim \mathcal{U}[1, 1.2]^3 \quad \text{defines uncertainty in Young's modulus}$$
$$x = \text{position}$$
$$\mu(x) = \mathbb{E}[g(\mathbf{Z}, x)] = \int_{[0,1]^3} g(\mathbf{z}, x)\, \mathrm{d}\mathbf{z} \approx \frac{1}{n} \sum_{i=1}^{n} g(\mathbf{Z}_i, x)$$
$$\mu(\text{end}) = 1037$$



[5] M. Parno and L. Seelinger (2022). *Uncertainty propagation of material properties of a cantilevered beam*. URL: https://um-bridge-benchmarks.readthedocs.io/en/docs/forward-benchmarks/muq-beam-propagation.html.

IID vs. Low Discrepancy for the Cantilevered Beam via QMCPy[6]

$$g(\boldsymbol{Z}, x) = \text{beam deflection}$$

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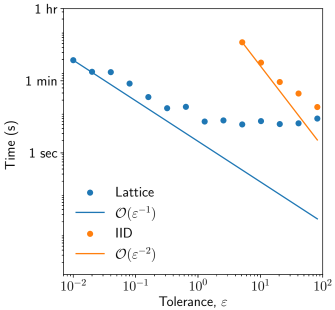

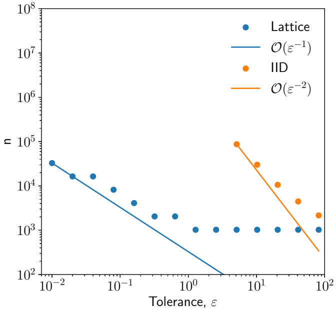

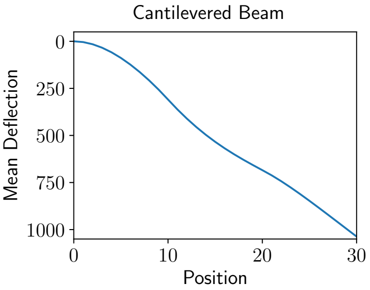

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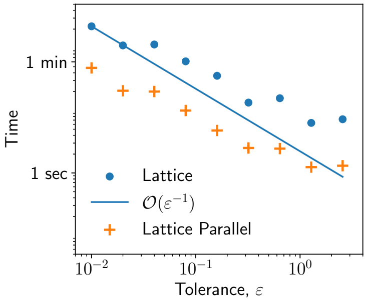

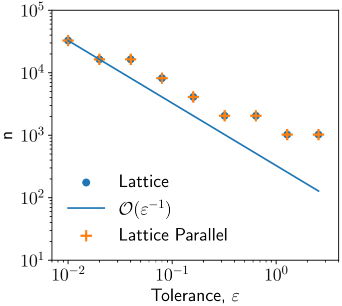

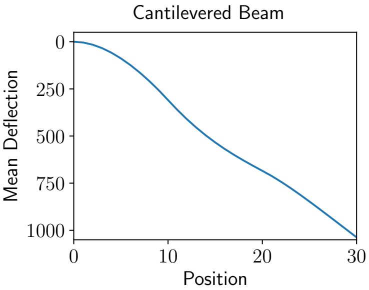

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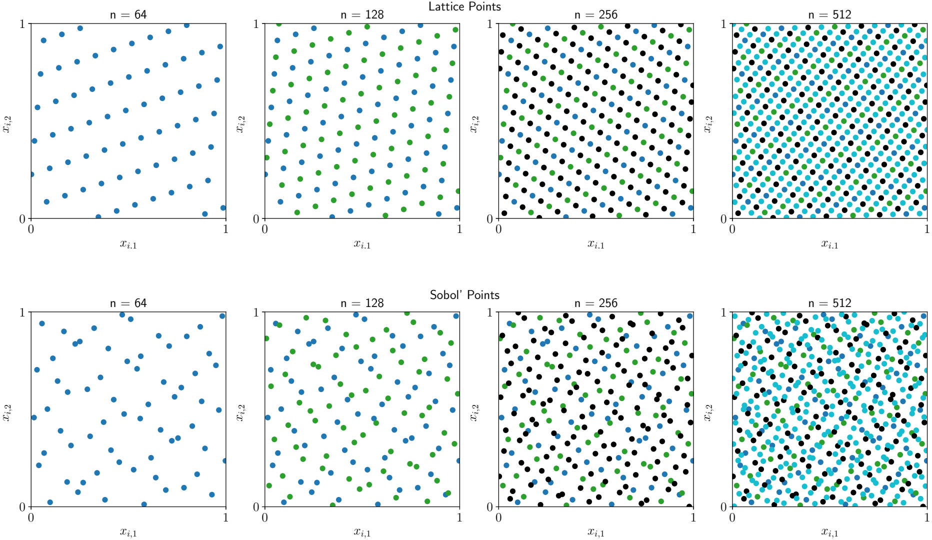
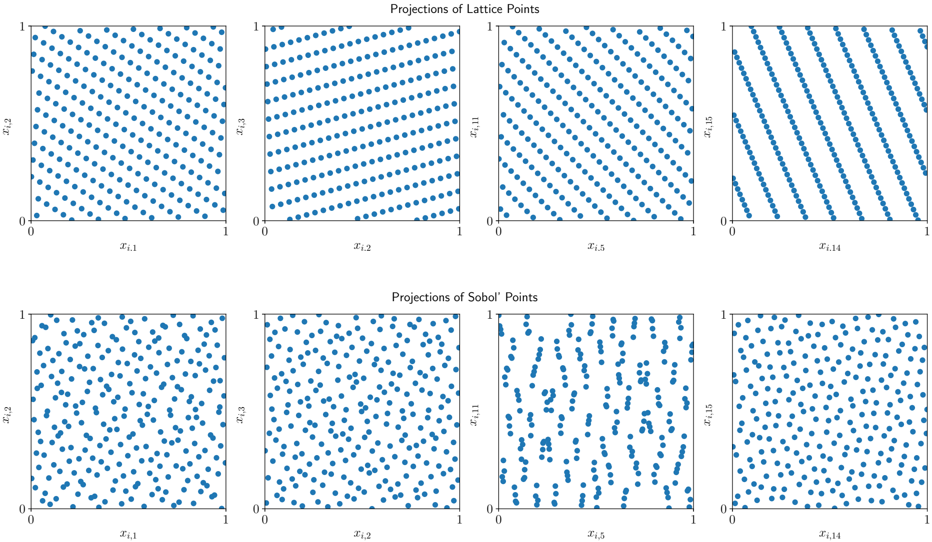
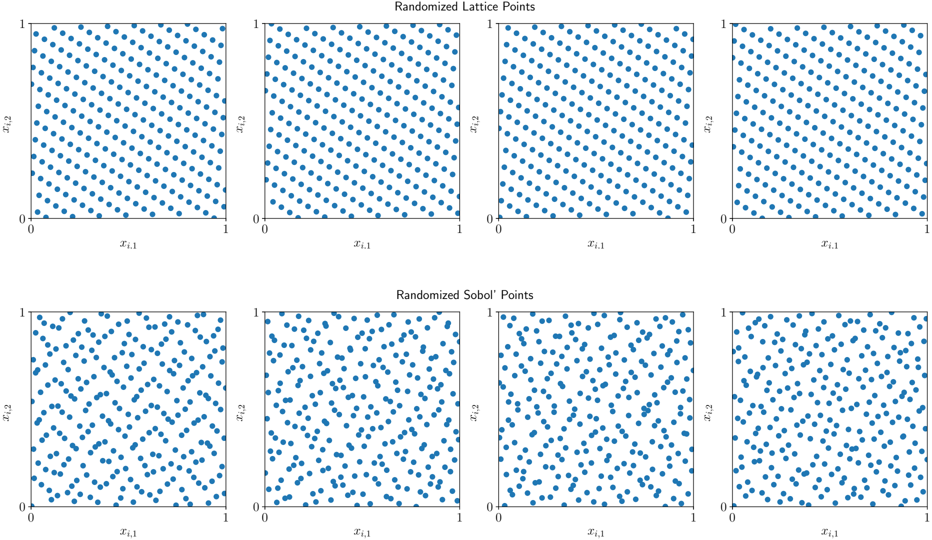
Low Discrepancy Points Fill Space



Low Discrepancy Points Look “Good” in All Coordinate Projections



Low Discrepancy Points Can Be Randomized



Lessons from the Trio Identity

$$\overbrace{\int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}^{\mathbb{E}[f(\boldsymbol{X})],\ \boldsymbol{X}\sim\mathcal{U}[0,1]^d} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i) = \mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{DSC}(\{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{VAR}(f)$$

- Use low discrepancy[7] instead of IID sampling for performance gains

[7] J. Dick, P. Kritzer, and F. Pillichshammer (2022). *Lattice Rules: Numerical Integration, Approximation, and Discrepancy*. Springer Series in Computational Mathematics. Springer Cham. DOI: https://doi.org/10.1007/978-3-031-09951-9; J. Dick, F. Kuo, and I. H. Sloan (2013). "High dimensional integration — the Quasi-Monte Carlo way". In: *Acta Numer.* 22, pp. 133–288. DOI: 10.1017/S0962492913000044; J. Dick and F. Pillichshammer (2010). *Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration*. Cambridge: Cambridge University Press.

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- Use low discrepancy[7] instead of IID sampling for performance gains
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[7] J. Dick, P. Kritzer, and F. Pillichshammer (2022). *Lattice Rules: Numerical Integration, Approximation, and Discrepancy*. Springer Series in Computational Mathematics. Springer Cham. DOI: `https://doi.org/10.1007/978-3-031-09951-9`; J. Dick, F. Kuo, and I. H. Sloan (2013). "High dimensional integration — the Quasi-Monte Carlo way". In: *Acta Numer.* 22, pp. 133–288. DOI: `10.1017/S0962492913000044`; J. Dick and F. Pillichshammer (2010). *Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration*. Cambridge: Cambridge University Press.

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- Use low discrepancy[7] instead of IID sampling for performance gains
- Randomize when possible so avoid bad $\mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n)$. Scrambled Sobol' often beats unscrambled Sobol' in order of convergence. Randomizing moves points off the boundaries.
- Error decay rate, $\mathrm{DSC}(\{\boldsymbol{x}\}_{i=1}^n)$, limited by the assumptions on f implicit in the choice of VAR
- Deterministic trio identities constrain $-1 \le \mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n) \le 1$ but may be pessimistic
- If $\mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n)$ is consistently small, look for a better choice of VAR and DSC

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- If $\mathrm{CNF}(f,\{\boldsymbol{x}\}_{i=1}^n)$ is consistently small, look for a better choice of VAR and DSC
- Theory explains how well an algorithm works; practice can help sharpen theory

[7] J. Dick, P. Kritzer, and F. Pillichshammer (2022). *Lattice Rules: Numerical Integration, Approximation, and Discrepancy*. Springer Series in Computational Mathematics. Springer Cham. DOI: https://doi.org/10.1007/978-3-031-09951-9; J. Dick, F. Kuo, and I. H. Sloan (2013). "High dimensional integration — the Quasi-Monte Carlo way". In: *Acta Numer.* 22, pp. 133–288. DOI: 10.1017/S0962492913000044; J. Dick and F. Pillichshammer (2010). *Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration*. Cambridge: Cambridge University Press.

Estimating or Bounding the Error from Simulation Data

$$\overbrace{\int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}}^{\mathbb{E}[f(\boldsymbol{X})],\ \boldsymbol{X}\sim\mathcal{U}[0,1]^d} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i) = \mathrm{CNF}(f, \{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{DSC}(\{\boldsymbol{x}\}_{i=1}^n)\ \mathrm{VAR}(f)$$

When to stop sampling because the error is small enough?

- $\mathrm{VAR}(f)$ is impractical to bound
- $\mathrm{DSC}(\{\boldsymbol{x}\}_{i=1}^n)$ is expensive to calculate

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Many do replications

$$\left|\int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i)\right|^2 \approx \frac{\text{fudge}^2}{R}\sum_{r=1}^{R}\left(\frac{1}{Rn}\sum_{q,i=1}^{R,n} f(\boldsymbol{x}_i^{(q)}) - \frac{1}{n}\sum_{i=1}^{n} f(\boldsymbol{x}_i^{(r)})\right)^2$$

where $\{\boldsymbol{x}_i^{(1)}\}_{i=1}^n, \ldots \{\boldsymbol{x}_i^{(R)}\}_{i=1}^n$ are randomizations of a low discrepancy sequence.

Estimating or Bounding the Error from Simulation Data

For $\left\{\begin{matrix}\text{lattice}\\ \text{Sobol'}\end{matrix}\right\}$ or sampling

$$\left| \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \frac{1}{n}\sum_{i=0}^{n} f(\boldsymbol{x}_i) \right| \le \sum_{\boldsymbol{k}\in\text{dual lattice}} \left|\widehat{f}(\boldsymbol{k})\right|$$

where $\widehat{f}(\boldsymbol{k})$ are the Fourier $\left\{\begin{matrix}\text{complex exponential}\\ \text{Walsh}\end{matrix}\right\}$ coefficients of f and the dual lattice consists of wave numbers of $\left\{\begin{matrix}\text{complex exponential}\\ \text{Walsh}\end{matrix}\right\}$ bases that are perfectly aliased with 1.

Rigorous data-driven error bounds based on sums of discrete Fourier $\left\{\begin{matrix}\text{complex exponential}\\ \text{Walsh}\end{matrix}\right\}$ coefficients of f are valid for not too noisy/peaky f[8].

[8] F. J. H. and Ll. A. Jiménez Rugama (2016). "Reliable Adaptive Cubature Using Digital Sequences". In: *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Leuven, Belgium, April 2014*. Ed. by R. Cools and D. Nuyens. Vol. 163. Springer Proceedings in Mathematics and Statistics. arXiv:1410.8615 [math.NA]. Springer-Verlag, Berlin, pp. 367–383; Ll. A. Jiménez Rugama and F. J. H. (2016). "Adaptive Multidimensional Integration Based on Rank-1 Lattices". In: *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Leuven, Belgium, April 2014*. Ed. by R. Cools and D. Nuyens. Vol. 163. Springer Proceedings in Mathematics and Statistics. arXiv:1411.1966. Springer-Verlag, Berlin, pp. 407–422.

Estimating or Bounding the Error from Simulation Data

Data-driven error bounds based on credible intervals assume that f is an instance of a Gaussian process whose parameters are tuned; valid for f that are not outliers. Computation is fast if covariance kernel matches the sample[8].

[8] R. Jagadeeswaran and F. J. H. (2019). “Fast Automatic Bayesian Cubature Using Lattice Sampling”. In: *Stat. Comput.* 29, pp. 1215–1229. DOI: 10.1007/s11222-019-09895-9; R. Jagadeeswaran and F. J. H. (2022). “Fast Automatic Bayesian Cubature Using Sobol’ Sampling”. In: *Advances in Modeling and Simulation: Festschrift in Honour of Pierre L’Ecuyer*. Ed. by Z. Botev, A. Keller, C. Lemieux, and B. Tuffin. Springer, Cham, pp. 301–318. DOI: 10.1007/978-3-031-10193-9_15.

Problems Involving Several Integrals

$$\text{posterior mean}_j = \frac{\int_{\mathbb{R}^d} x_j \,\text{likelihood}(\boldsymbol{x}, \text{data})\, \text{prior}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}}{\int_{\mathbb{R}^d} \text{likelihood}(\boldsymbol{x}, \text{data})\, \text{prior}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}}, \qquad j = 1, \ldots, d$$

$$\text{expected output}(\boldsymbol{s}) = \mathbb{E}[\text{output}(\boldsymbol{s}, \boldsymbol{X})] = \int_{\mathbb{R}^d} \text{output}(\boldsymbol{s}, \boldsymbol{x})\, \varrho(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}, \qquad \boldsymbol{s} \in \Omega$$

$$\text{sensitivity index}_j = \int_{[0,1]^{2d}} f(\boldsymbol{x})[f(x_j, \boldsymbol{z}_{-j}) - f(\boldsymbol{z})] \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{z}, \qquad j = 1, \ldots, d$$

Stopping criteria have been extended to these cases[9]

[9] F. J. H., Ll. A. Jiménez Rugama, and D. Li (2018). “Adaptive Quasi-Monte Carlo Methods for Cubature”. In: *Contemporary Computational Mathematics — a celebration of the 80th birthday of Ian Sloan*. Ed. by J. Dick, F. Y. Kuo, and H. Woźniakowski. Springer-Verlag, pp. 597–619. DOI: 10.1007/978-3-319-72456-0; A. G. Sorokin and R. Jagadeeswaran (2023+). “Monte Carlo for Vector Functions of Integrals”. In: *Monte Carlo and Quasi-Monte Carlo Methods: MCQMC, Linz, Austria, July 2022*. Ed. by A. Hinrichs, P. Kritzer, and F. Pillichshammer. Springer Proceedings in Mathematics and Statistics. submitted for publication. Springer, Cham.

Bayesian Logistic Regression for Cancer Survival Data

$$\mathrm{logit}(\text{probability of } 5 \text{ year survival}) = \beta_0 + \beta_1\text{patient age} + \beta_2\text{operation year} + \beta_3\text{\# positive axillary nodes}$$

Logistic regression to estimate β_j from 306 data[10] with error criterion of

$$\text{absolute error} \le 0.05 \ \& \ \text{relative error} \le 0.5$$

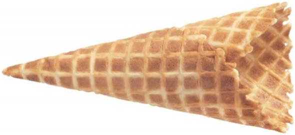
method	β_0	β_1	β_2	β_3	$\frac{\text{all true}}{\text{all}}$	$\frac{\text{true pos}}{\text{all pos}}$	$\frac{\text{true pos}}{\text{true pos} + \text{false neg}}$
Bayesian & qmcpy	0.0080	-0.0041	0.1299	-0.1569	74%	74%	100%
elastic net	0.0020	-0.0120	0.0342	-0.11478	74%	77%	93%

[10] SJ Haberman (1976). *Generalized residuals for log-linear models, proceedings of the 9th International Biometrics Conference*.

Lessons from Data-Based Error Bounds

$$\left| \int_{[0,1]^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} - \frac{1}{n} \sum_{i=0}^{n} f(\boldsymbol{x}_i) \right| \le \text{some function of } \{(\boldsymbol{x}_i, f(\boldsymbol{x}_i))\}_{i=1}^{n}$$

- Theoretical bounds are impractical
- Every data-based error bound can be fooled
- There are better choices than random replications

$f \in$  not 

Importance Sampling and Control Variates

The original problem may look like

$$\int_{\Omega} g(\boldsymbol{t}) \, \mathrm{d}\boldsymbol{t}$$

$$\text{but needs to become} = \int_{[0,1]^d} f(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$$

Importance Sampling and Control Variates

To facilitate and expedite its solution, one may

- perform a variable transformation, equivalent to importance sampling[11], and/or
- subtract a trend (control variate)[12] with integral zero

$$\int_{\Omega} g(\boldsymbol{t})\,\mathrm{d}\boldsymbol{t} \underbrace{=}_{\boldsymbol{t}=\boldsymbol{\Psi}(\boldsymbol{x})} \int_{[0,1]^d} g(\boldsymbol{\Psi}(\boldsymbol{x})) \left|\frac{\partial \boldsymbol{\Psi}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right| \mathrm{d}\boldsymbol{x}, \qquad \boldsymbol{T} = \boldsymbol{\Psi}(\boldsymbol{X}) \sim \left[\left|\frac{\partial \boldsymbol{\Psi}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right|_{\boldsymbol{x}=\boldsymbol{\Psi}^{-1}(\boldsymbol{t})}\right]^{-1}$$

$$= \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

[11] A. B. Owen and Y. Zhou (2000). "Safe and Effective Importance Sampling". In: *J. Amer. Statist. Assoc.* 95, pp. 135–143.

[12] F. J. H., C. Lemieux, and A. B. Owen (2005). "Control Variates for Quasi-Monte Carlo". In: *Statist. Sci.* 20, pp. 1–31. DOI: 10.1214/088342304000000468.

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$$= \int_{[0,1]^d} \left[g(\boldsymbol{\Psi}(\boldsymbol{x})) \left| \frac{\partial \boldsymbol{\Psi}(\boldsymbol{x})}{\partial \boldsymbol{x}} \right| - h(\boldsymbol{x}) \right] \mathrm{d}\boldsymbol{x} = \int_{[0,1]^d} f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

to make $\mathrm{VAR}(f)$ smaller. Choosing $\boldsymbol{\Psi}$ and h is more art than science.

[11] A. B. Owen and Y. Zhou (2000). "Safe and Effective Importance Sampling". In: *J. Amer. Statist. Assoc.* 95, pp. 135–143.

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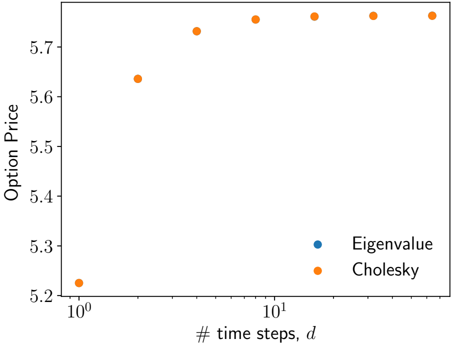
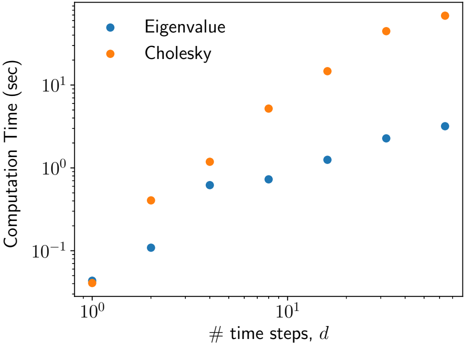
Asian Option Pricing

- Option payoff is function of a stock price path modeled by a stochastic differential equation
- Option price is expected value of payoff
- True answer is the limit as # of time steps, d, goes to ∞
- Ψ based on the eigenvector-eigenvalue decomposition of the covariance matrix is more efficient than the Cholesky decomposition





Multilevel methods[13]

Large or infinite d when discretizing a continuous stochastic process. Write as

$$\lim_{d\to\infty}\int_{[0,1]^d} f_d(\boldsymbol{x}_d)\,\mathrm{d}\boldsymbol{x}_d = \overbrace{\int_{[0,1]^{d_1}} f_{d_1}(\boldsymbol{x}_{d_1})\,\mathrm{d}\boldsymbol{x}_{d_1}}^{\text{low dimensional approximation}} + \overbrace{\int_{[0,1]^{d_2}} [f_{d_2}(\boldsymbol{x}_{d_2}) - f_{d_1}(\boldsymbol{x}_{d_1})]\,\mathrm{d}\boldsymbol{x}_{d_2}}^{\text{improvement}} + \cdots$$

$$+ \int_{[0,1]^{d_L}} [f_{d_L}(\boldsymbol{x}_{d_L}) - f_{d_{L-1}}(\boldsymbol{x}_{d_{L-1}})]\,\mathrm{d}\boldsymbol{x}_{d_L} + \lim_{d\to\infty}\int_{[0,1]^d} f_d(\boldsymbol{x}_d)\,\mathrm{d}\boldsymbol{x}_d - \int_{[0,1]^{d_L}} f_{d_L}(\boldsymbol{x}_{d_L})\,\mathrm{d}\boldsymbol{x}_{d_L}$$

$$\approx \underbrace{\frac{1}{n_1}\sum_{i=1}^{n_1} f_{d_1}(\boldsymbol{x}_{i,d_1}^{(1)})}_{\text{cheap since } d_1 \text{ small}} + \frac{1}{n_2}\sum_{i=1}^{n_2}[f_{d_2}(\boldsymbol{x}_{i,d_2}^{(2)}) - f_{d_1}(\boldsymbol{x}_{i,d_1}^{(2)})] + \cdots + \underbrace{\frac{1}{n_L}\sum_{i=1}^{n_L}[f_{d_L}(\boldsymbol{x}_{i,d_L}^{(L)}) - f_{d_{L-1}}(\boldsymbol{x}_{i,d_{L-1}}^{(L)})]}_{\text{cheap since } n_L \text{ small}}$$

where $d_1 < \cdots < d_L$ and $n_1 > \cdots > n_L$. Evaluation of $f_d(\boldsymbol{x}_d)$ is typically $\mathcal{O}(d)$.

[13] M. Giles (2013). "Multilevel Monte Carlo methods". In: *Monte Carlo and Quasi-Monte Carlo Methods 2012*. Ed. by J. Dick, F. Y. Kuo, G. W. Peters, and I. H. Sloan. Vol. 65. Springer Proceedings in Mathematics and Statistics. Springer-Verlag, Berlin. DOI: 10.1007/978-3-642-41095-6.

Message

Problems in Bayesian inference, uncertainty quantification, quantitative finance, (high energy) physics, etc. require numerically evaluating

$$\underbrace{\mathbb{E}[f(\boldsymbol{X})]}_{\text{expectation}} = \underbrace{\int_{\Omega} f(\boldsymbol{x})\, \varrho(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}}_{\text{integral}}, \qquad \boldsymbol{X} \sim \varrho$$

There is value in

- low discrepancy sampling, aka quasi-Monte Carlo methods
- data-driven error bounds
- flattening and reducing the effective dimension of the integrand
- quality quasi-Monte Carlo software like qmcpy
- physicists and quasi-Monte Carlo theorists collaborating more

Slides at `speakerdeck.com/fjhickernell/argonne2023maytalk`

Jupyter notebook with computations and figures here. Visit us at `qmcpy.org`

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