Applicability of Quasi-Monte Carlo for lattice systems

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Outline

Motivation

The (An)Harmonic Oscillator on the Lattice

Results

Outlook/Conclusions

typical lattice problem:

$$Z = \int \mathcal{D}x \; e^{-S[x]} \; ; \quad x = (x_1, \ldots, x_d) \tag{1}$$

$$\langle O \rangle = Z^{-1} \int \mathcal{D}x \; e^{-S[x]} \; O[x] \tag{2}$$

- stochastic approximation through Markov chain Monte Carlo methods: Metropolis algorithm, HMC , ...
- finite Markov chain: $x_1, \ldots, x_N \to N$ samples of O: $O_1, \ldots, O_N$
- O_i random variables with variance σ_O^2
- estimate $\overline{\langle O \rangle} = \frac{1}{N} \sum_{i=1}^{N} O_i$ has standard error

$$\Delta \overline{\langle O \rangle} = \frac{\sigma_O}{\sqrt{N}}$$

- need 100 times more statistics to get additional digit of precision
- past improvements: reduce σ_O and auto-correlation
- Improved error scaling would be highly desirable!

improved error scaling?

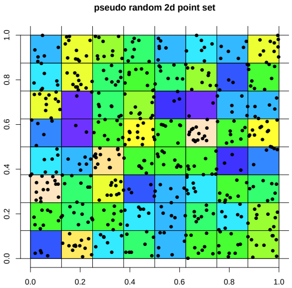
quasi-Monte Carlo (QMC) is an approach to improve the asymptotic error behaviour
see for example F. Kuo, Ch. Schwab and I. Sloan, 2012[KSS12]

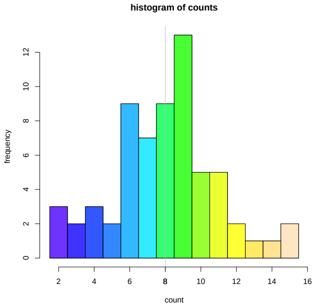
- construction of deterministic low-discrepancy point-sets in arbitrary many dimensions
- low-discrepancy $\rightarrow$ "more uniform" (see below)
- promises N^{-1} asymptotic error behaviour for integrands with certain properties (e.g. Gaussian)
- $\rightarrow$ **two** times more digits with the same number of samples!!
- applied successfully to financial problems (see bibliography)

QMC point sets are more uniform

How does an actual uniform sampling in two dimensions look like?

Example: 512 two-dimensional pseudo-random points





- sample 512 points
- introduce grid of 8×8 equal squares
- count number of points in each square
- count occurrence of $1, 2, \ldots$ points in a square (histogram of histogram)

- $\approx$ Poisson distribution with $\lambda = \bar{n} = 8$
- uneven sampling $\rightarrow$ larger stochastic error

QMC point set (2d Sobol samples) :

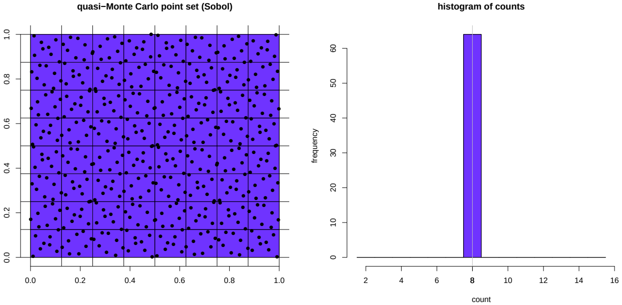


Figure: 512 uniform 2d Sobol points

- each square contains same number of points $\rightarrow$ delta distribution
- even coverage
- less stochastic fluctuations
- simulate effect of higher statistics with much less samples
- in this sense QMC is exactly what we want
- randomisation possible (RQMC) w/o changing properties $\rightarrow$ practical error estimation

problem description

lattice action (see "Creutz and Freedman" [CF81]):

$$S = a \sum_{i=1}^{d} \left(\frac{M_0}{2} \frac{(x_{i+1} - x_i)^2}{a^2} + \frac{\mu^2}{2} x_i^2 + \lambda x_i^4 \right) \; ; \quad x_{d+1} = x_1 \quad \text{(p.b.)}$$

$M_0 \ldots$ particle mass

$\mu^2 = M_0 \omega^2 \ldots$ frequency/spring constant

$a \ldots$ lattice spacing

$d \ldots$ number of lattice sites $\rightarrow T = da \ldots$ time extent

- $\lambda = 0 \rightarrow$ harmonic oscillator
- $\lambda > 0 \rightarrow$ anharmonic oscillator, $\mu^2 < 0 \rightarrow$ double well potential

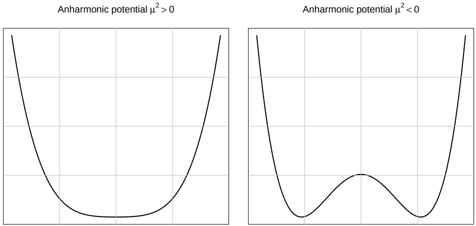


Figure: two cases for the anharmonic potential

observables

primary observables

$$\langle x^2 \rangle = \langle \frac{1}{d} \sum_i x_i^2 \rangle \tag{3}$$

$$\langle x^4 \rangle = \langle \frac{1}{d} \sum_i x_i^4 \rangle \tag{4}$$

$$\langle x_k x_{k+j} \rangle = \langle \frac{1}{d} \sum_i x_i x_{i+j} \rangle \ldots \text{correlator} \tag{5}$$

derived quantities

$$E_0 = 3\lambda \langle x^4 \rangle + \mu^2 \langle x^2 \rangle + \frac{\mu^4}{16} \tag{6}$$

$$E_1 - E_0 = \text{energy gap from correlator fit} \tag{7}$$

theoretically known for $a \to 0$, $T = da \to \infty$ (iterative method)
Blankenbecler, DeGrand and Sugar 1980 [BDS80]

experiment I: harmonic oscillator ($\lambda = 0$, $\mu^2 > 0$)

partition function can be written as multivariate Gaussian integral

$$Z = \int \mathcal{D}x \exp\left(-\frac{1}{2}x^t C^{-1} x\right) \tag{8}$$

$$C^{-1} = \frac{2M_0}{a}\left((1 + \frac{a^2\mu^2}{2M_0})\delta_{ij} - \frac{1}{2}(\delta_{ij+1} + \delta_{ij-1})\right) \tag{9}$$

covariance matrix: $C = SDS^t \to D = diag(\beta_1, \ldots, \beta_d) \quad \beta_i \in \mathbb{R}^+$

$$x = Sw \quad \Rightarrow \quad Z \to \int \mathcal{D}w \exp\left(-\sum_i \frac{1}{2\beta_i} w_i^2\right) \tag{10}$$

$\to$ sampling algorithm

- generate uniform $z \in [0,1]^d$ (pseudo random / QMC)
- $w_i = \sqrt{\beta_i}\Phi^{-1}(z_i)$, Φ^{-1} ... inverse standard normal CDF
  - ordering of eigenvalues $\beta_1 > \beta_2 > \ldots > \beta_d$ when using QMC
  - like ordering of importance $z_1 > z_2 > \ldots > z_d$
- $x_i = S_{ij} w_j$ (Hartley transformation, involutive: $S = S^{-1} = S^t$)

harmonic oscillator results

parameters: $\mu^2 = 2.0$, $M_0 = 0.5$, $a = 0.5$ & $d = 100$

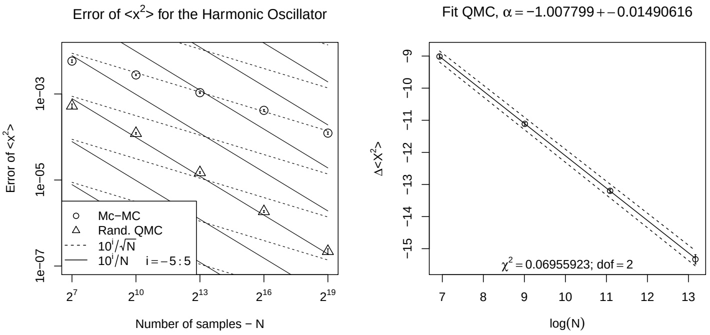


Figure: left: asymptotic error behaviour of MC/QMC, right: fit of QMC error $\sim N^{\alpha}$

- $\rightarrow$ QMC at work
- trivial, but successful application to physical problem

experiment II: anharmonic oscillator ($\lambda = 1$, $\mu^2 < 0$)

direct sampling not possible because of anharmonic part of the potential
$\rightarrow$ do reweighting

$$Z = \int \mathcal{D}x \exp\left(-\frac{1}{2}x^t C^{-1} x - a\lambda \sum_i x_i^4\right) \tag{11}$$

C^{-1} indefinite ($\mu^2 < 0$) $\rightarrow$ define $C_{sim}^{-1} = \frac{2M_0}{a}\left((1 + \mu^2_{\mathbf{sim}}\frac{a^2}{2M_0})\delta_{ij} - \frac{1}{2}\left(\delta_{ij+1} + \delta_{ij-1}\right)\right)$
with $\mu^2_{sim} > 0$, arbitrary insert the "productive 0"

$$Z = \int \mathcal{D}x \exp\left(\underbrace{-\frac{1}{2}x^t C_{sim}^{-1} x}_{\text{sampling}} \underbrace{-\frac{1}{2}x^t(C^{-1} - C_{sim}^{-1})x - a\lambda \sum_i x_i^4}_{\text{reweighting}}\right) \tag{12}$$

$$= \int \mathcal{D}x \; e^{-\frac{1}{2}x^t C_{sim}^{-1} x} \; W(x) \tag{13}$$

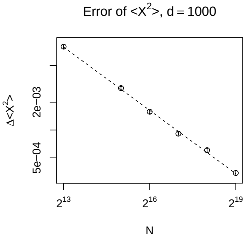
$\rightarrow$ sampling like harmonic oscillator but with $C \rightarrow C_{sim}$ observable estimation from samples $(x^j)_{j=1,\ldots,N}$:

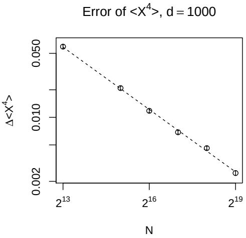
$$\langle O \rangle \approx \frac{\sum_j W(x^j) O(x^j)}{\sum_j W(x^j)} \quad W(x) = e^{-\frac{1}{2}\cdots}$$

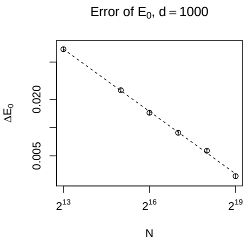
numerical results/anharmonic oscillator

parameters: $M_0 = 0.5$, $a = 0.015$, $\mu^2 = -16$
fit: $\Delta O \sim CN^{\alpha}$

	O	α	$\log C$	χ^2/dof
$d = 100$	X^2	-0.763(8)	2.0(1)	7.9 / 6
	X^4	-0.758(8)	4.0(1)	13.2 / 6
	E_0	-0.737(9)	4.0(1)	8.3 / 6
$d = 1000$	X^2	-0.758(14)	2.0(2)	5.0 / 4
	X^4	-0.755(14)	4.0(2)	5.7 / 4
	E_0	-0.737(13)	4.0(2)	4.0 / 4







(arXiv:1302.6419 , K. Jansen, H. Leovey, A. Ammon, A. Griewank, M. Müller-Preußker, 2013[JLA$^+$13])

energy gap

- asymptotic behaviour of correlator
- non-trivial observable
- not possible to detect on present parameter setup (T too small)
- changed $\mu^2 = -16 \rightarrow \mu^2 = -4$,
- energy gap: $0.0015 \rightarrow 1.576$

result obtained for $d = 100$, $N = 2^5, 2^8, 2^{11}, 2^{14}$ and 400 Sobol' sequences each:

$$\alpha = -0.735(13)$$

(Tobias Hartung, 2013, personal communication)

outlook & conclusions

- harmonic oscillator: QMC works perfectly (as expected)
- anharmonic oscillator: significantly improved error scaling $\to N^{-\frac{3}{4}}$

  remaining questions:
  - Why do we observe this $N^{-\frac{3}{4}}$ behaviour??
  - further improvements by generalised choice of C_{sim}?
  - other, possibly non-Gaussian, sampling methods
- next step: one-dimensional spin model in cosine discretisation

$$S[\phi] = Ia \sum_i -\frac{1}{a^2} cos(\phi_{i+1} - \phi_i) \tag{14}$$

study χ_Q (topological susceptibility) and $\Delta E = E_1 - E_0$ (energy gap)

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