# High dimensional integration of kinks and jumps – smoothing by preintegration


YACHAY TECH

SCHOOL OF MATHEMATICS SCIENCES AND INFORMATION TECHNOLOGY

Andreas Griewank and Hernan Leövey

with thanks to co-authors
F. Kuo and I. Sloan


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$$\text{To approximate improper integral } I\,f \;=\; \int_{\mathbb{R}^{1+d}} f(x)\rho(x)dx \quad \text{with } d \geq 50$$

$$\text{define sample sequence} \quad X \;=\; \{x_k\}_{k=1}^{\infty} \quad \text{and set}$$

$$I\,f \approx Q_n f \;\equiv\; \frac{1}{n}\sum_{k=1}^{n} f(x_k)$$

For true random choice $X =$ Monte Carlo (MC) w.r.t. probability density $\rho$

$$\mathbb{E}|Q_n f - I\,f| \quad \sim \quad 1/\sqrt{n}$$

Not so random choice $X =$ Quasi-Monte Carlo (QMC) leads to

$$\mathbb{E}|Q_n f - I\,f| \quad \sim \quad 1/n^{(1-\delta)}$$

where $\delta \geq 0$ depends on method and function *smoothness*.

# Not so smooth Example

Path-dependent option pricing problems need high-dimensional numerical integration, but don't fit the theory: options become worthless if the final asset value is below the **strike price** $K$.
So the integrand in the expected value of the payoff looks like

$$f \;=\; \max\left\{\text{value} - K, 0\right\}.$$

Because of the max function, the integrand does not lie in any mixed derivative function space, as the theory assumes for both Quasi-Monte Carlo (QMC) and sparse grid methods.

# The smoothing Mechanism

The following 2-dimensional example is a simplified model of the Asian option pricing problem, with $1 + d = 2$. We call the variables $x$ and $y$ instead of $x_0$ and $x_1$.

$$f(x, y) = \max(\varphi(x, y), 0) \quad \text{where} \quad \varphi(x, y) = \mathrm{e}^x - y,$$

Thus $\frac{\partial \varphi}{\partial x} = \mathrm{e}^x > 0$, and $\varphi \to \infty$ as $x \to \infty$. Consequently:

$$\int_{-\infty}^{\infty} \max(\mathrm{e}^x - y, 0) \exp\left(-\tfrac{1}{2}x^2\right)\mathrm{d}x$$

$$= \int_{\log y}^{\infty} (\mathrm{e}^x - y) \exp\left(-\tfrac{1}{2}x^2\right)\mathrm{d}x.$$

which is a perfectly smooth function in $y$.

# Some related publications

1. M. Griebel, F. Kuo, I. Sloan, Math Comp 2013 and Note (2016)
2. X. Wang (2015)
3. P. Glasserman and J. Staum (2001)
4. N. Achtsis, R. Cools, and D. Nuyens (2013)
5. D. Nuyens and B. J. Waterhouse (2012)
6. J.H. Chan and M. Joshi (2015)
7. R. Tempone
8. Ch. Bayer
9. M. Siebenlogen
10. ...

Consider

$$I \equiv \int_{\mathbb{R}^{1+d}} \left(f(x_0, x)\rho(x_0)\, dx_0\right) \rho_d(x) dx \quad \text{with} \quad x \in \mathbb{R}^d$$

where

$$f(x_0, x) = \max(0, \theta(x_0, x)) = \theta(x_0, x)\, \mathrm{ind}(\theta(x_0, x))$$

or more generally we may also allow jumps by setting

$$\boxed{f(x_0, x) = \theta(x_0, x)\, \mathrm{ind}(\varphi(x_0, x))}$$

with $C^r$ smooth $\theta$ and *switching function* $\varphi : \mathbb{R}^{1+d} \mapsto \mathbb{R}$.

## Monotonicity assumption w.r.t. $x_0$

$$D_0\varphi(x_0,x) \;\equiv\; \frac{\partial}{\partial x_0}\varphi(x_0,x) \;>\; 0 \quad \textit{and} \quad \lim_{x_0\to\infty}\varphi(x_0,x) \;=\; \infty$$

implies existence of *boundary function*

$$\psi(x) \;=\; \sup\{x_0 \in \mathbb{R} : \varphi(x_0,x) = 0\} \;:\; \mathbb{R}^d \to \{-\infty\} \cup \mathbb{R}$$

## Lemma

$\psi$ is (extended) continuous and belongs to $C^r(\mathcal{U})$ on open

$$\mathcal{U} \equiv \{x \in \mathbb{R}^d : \psi(x) > -\infty\}$$

with closed complement $\mathcal{U}_+ = \mathcal{U}^c$.

# Projection Operator

## Consequence of Fubini

$$I\,f \;\equiv\; \int_{\mathbb{R}^d} (P_\psi\theta)(x)\rho_d(x)\,dx$$

where

$$(P_\psi\theta)(x) \;\equiv\; \int_{-\infty}^{\infty} f(x_0, x)\rho(x_0)dx_0$$

$$= \int_{\psi(x)}^{\infty} \theta(x_0, x)\rho(x_0)dx_0 \;:\; \mathcal{L}_{1+d,1,\rho_{d+1}} \to \mathcal{L}_{d,1,\rho_d}$$

## Idea

Sample $x \in X \subset \left(\mathbb{R}^d\right)^n$ and evaluate Projection $P_\psi\theta(x) \in \mathbb{R}$ 'exactly'.

# Desirable Properties of Projection

- variance reduction, i.e. $\sigma^2(P_\psi\theta) = \sigma^2(f)(1 - Sob_0(f)^2)$ ✓
- continuous differentiability, i.e. $P_\psi\theta \in C^r(\mathbb{R}^d)$ ✓
- bounded Sobolev norm, i.e. $P_\psi\theta \in \mathcal{W}^r_{d,p,\rho_d}$ ✓
- membership in tensor space, i.e. $P_\psi\theta \in \mathcal{W}^d_1$ (✓)
- boundedness in suitable norm, i.e. $|||P_\psi\, \theta|||_? \leq c_\psi \|\theta\|_?$

For a function $f \in \mathcal{L}_{1+d,2,\rho_{1+d}}$, the ANOVA decomposition is

$$f(x) = \sum_{\mathfrak{u} \subseteq \mathcal{D} \equiv \{0,1,2,\dots,d\}} f_{\mathfrak{u}}(x_{\mathfrak{u}}) \quad \text{with} \quad \mathbf{x}_{\mathfrak{u}} = (x_j)_{j \in \mathfrak{u}}$$

$$\Longrightarrow$$

$$P_\psi f_{\mathfrak{u}} = 0 \quad \text{if} \quad 0 \in \mathfrak{u}, \quad \text{whereas} \quad P_\psi f_{\mathfrak{u}} = f_{\mathfrak{u}} \quad \text{if} \quad 0 \notin \mathfrak{u}.$$

Since $f_{\mathfrak{u}}$ and $f_{\mathfrak{v}}$ are $L_{2,\rho_{1+d}}$-orthogonal if $\mathfrak{u} \neq \mathfrak{v}$ we get

$$\begin{aligned} \sigma^2(f) &= \sum_{\emptyset \neq \mathfrak{u} \subseteq \mathcal{D}} \sigma^2(f_{\mathfrak{u}}) \\ &= \underbrace{\sum_{\emptyset \neq \mathfrak{u} \subseteq \mathcal{D} \setminus \{0\}} \sigma^2(f_{\mathfrak{u}})}_{\sigma^2(P_\psi \theta)} + \underbrace{\sum_{\{0\} \in \mathfrak{u} \subseteq \mathcal{D}} \sigma^2(f_{\mathfrak{u}})}_{Sob_0^2(f)\sigma^2(f)} \end{aligned}$$

By extended Leibniz for $x \in \mathcal{U}$

$$D_k P_\psi \theta(x) \;=\; P_\psi(D_k\theta)(x) + \theta(\psi(x), x) D_k\psi(x)\rho(\psi(x))$$

where by implicit function theorem

$$D_k\psi(x) \;=\; -D_k\varphi(\psi(x), x))/D_0(\psi(x), x)$$

Repeated differentiation [see (griebel, kuo, sloan)] yields terms of the form

$$h(x) \;\equiv\; \frac{(D^\tau\theta)(\psi(x), x)\;\prod_{i=1}^{a}[(D^{\alpha^{(i)}}\varphi)(\psi(x), x)]}{[(D_0\varphi)(\psi(x), x)]^b}\,\rho^{(c)}(\psi(x))$$

for suitable integers $a, b, c, \tau$ depending on $r$.

Key assumption: $\quad x \to x_* \notin \mathcal{U} \implies h(x) \to 0 \qquad (1)$

# Example with nonsmooth boundary $\delta\mathcal{U}$ with $1 + d = 2$

$$\varphi(x_0, x) \;=\; \exp(x_0) - x_+^m sin(1/x_+) \quad \text{with} \quad z_+ \equiv \max(0, z)$$

$$\Longrightarrow$$

$$x_0 \;=\; \psi(x) = m\log(x_+) + \log(\sin(1/x_+)_+) : \mathbb{R} \to \{-\infty\} \cup \mathbb{R}$$

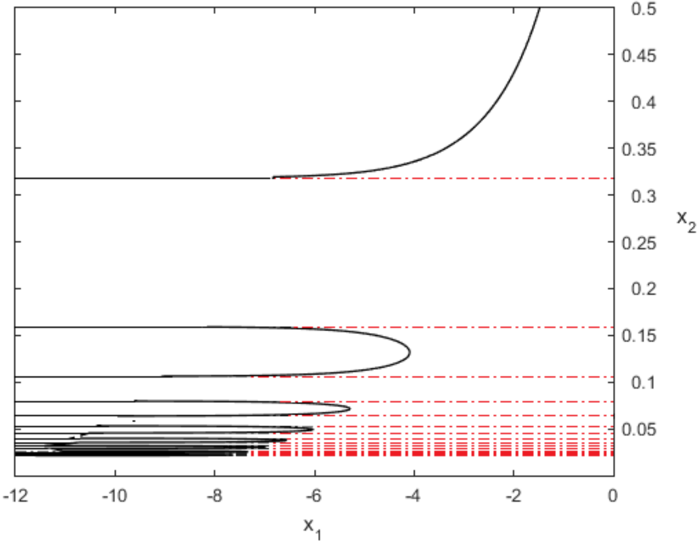
Regular domain:

$$\mathcal{U} = \frac{1}{\pi} \bigcup_{k \in N} \left(\frac{1}{2k+1}, \frac{1}{2k}\right) \cup \left(\frac{1}{\pi}, \infty\right)$$

Complement:

$$\mathcal{U}_+ = (-\infty, 0] \cup \frac{1}{\pi} \bigcup_{k \in N} \left[\frac{1}{2k}, \frac{1}{2k-1}\right]$$

# Nonsmooth Boundary Representation



## Lemma

*Suppose* $g \in C^r(U)$ *for some open domain* $U \subset \mathbb{R}^d$ *and that for all* $\alpha \in N_0^d$ *with* $|\alpha| \leq r$

$$U \ni x \to x_* \notin U \quad \Rightarrow \quad D^\alpha g(x) \to 0 \; .$$

*Then setting* $g(x) = 0$ *for* $x \notin U$ *we obtain* $g \in C^r(\mathbb{R}^n)$ *with* $D^\alpha(x) = 0$ *for all* $x \notin U$*.*

## Proof.

By induction on $\alpha$. Segments $\{x_* + \tau e_i\}_{0 \leq \tau \leq \bar{\tau}}$ intersect $\mathcal{U}$ on countable union of open interval, mean value theorem can be applied to $D^\alpha g$ on last one or in limit to show $D^\alpha g(x_* + \bar{\tau} e_i) = o(\bar{\tau})$. □

Proposition

*Provided (1) holds for all relevant $h(x)$ then*

$$\theta, \varphi \in C^r(\mathbb{R}^{1+d}), \rho_0 \in C^{r-1}(\mathbb{R}) \quad \Longrightarrow \quad P_\psi \theta \in C^r(\mathbb{R}^d)$$

(By Lemma applied to $g = P_\psi - P_{-\infty}$ which vanishes identially on $U_+$.)

Lemma (Hernan: (1) holds if)

$$\left| \frac{(D^\eta \theta)(x_0, x) \prod_{i=1}^a [(D^{\gamma^{(i)}} \varphi)(x_0, x)]}{[(D_0 \varphi)(x_0, x)]^b} \rho^{(c)}(x_0) \right| \leq E_0(x_0) E(x), \qquad (2)$$

*where $E_0, E$ are positive functions satisfying*

- *$E_0$ is bounded and $E_0(x_0) \to 0$ as $x_0 \to -\infty$,*
- *$E$ is locally bounded and p-integrable.*

$$\left| \frac{(D^{\tau}\theta)(x_0,x)\ \prod_{i=1}^{a}[(D^{\alpha^{(i)}}\varphi)(x_0,x)]}{[(D_0\varphi)(x_0,x)]^b}\ \rho_0^{(c)}(x_0) \right| \leq E_0(x_0)E(x)$$

where $E_0, E$ are positive functions satisfying

- $E_0$ is bounded and $E_0(x_0) \to 0$ as $x_0 \to -\infty$,
- $E$ is locally bounded and $p$-integrable with respect to $\rho$.

Can be verified for Asian and Binary options due to Gaussian probability distributions.

### Sobolev space

with smoothness parameter $0 \leq r \in N_0$

$$\mathcal{W}^r_{d,p,\rho_d} = \left\{ f \,:\, D^\alpha f \in \mathcal{L}_{p,\rho_d}(\mathbb{R}^d) \quad \text{for all} \quad |\alpha| \leq r \right\},$$

or 'mixed' variant with $\alpha \leq \mathbf{r} \in N_0^d$

### Theorem: Under above differentability assumption

$$\theta \in \mathcal{W}^r_{1+d,p,(\rho\,\rho_0)} \quad \Longrightarrow \quad P_\psi \theta \in \mathcal{W}^r_{n,p,\rho}$$

provided (griebel, kuo, sloan) for relevant integers $a, b, c, \tau$ depending on $r$ we have $h(x) \in \mathcal{L}_{d,p,\rho_d}$. Follows from Hernan's Lemma, which applies for Asian and Binary options due to Gaussian probability distributions.

Example: BINARY arithmetic Asian option, with $d+1=256$ time steps. The **expected value of the payoff** is then a 256-dimensional Gaussian integral

$$\mathbb{E}(\mathcal{P}_{1+d}) = e^{-rT} \int_{\mathbb{R}^{1+d}} \frac{S(0)}{d} \sum_{i=0}^{d} \exp\left(\left(r - \frac{\sigma^2}{2}\right) t_i + \sigma y_i\right)$$

$$\times \mathrm{ind}\left(\frac{S(0)}{d} \sum_{i=0}^{d} \exp\left(\left(r - \frac{\sigma^2}{2}\right) t_i + \sigma y_i\right) - K\right) \frac{\exp(-\frac{1}{2}\mathbf{y}^\top \Sigma^{-1} \mathbf{y})}{\sqrt{(2\pi)^{(1+d)} \det(\Sigma)}}$$

where $\Sigma \in \mathbb{R}^{1+d} \times \mathbb{R}^{1+d}$ is the covariance matrix for the Brownian motion,

$$\Sigma_{i,j} = \min(t_i, t_j).$$

# Factorizing the covariance matrix - PCA

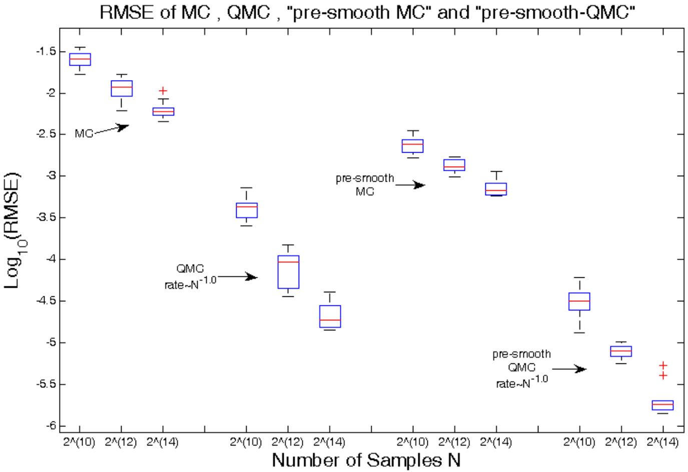
As usual we factorise $\Sigma = AA^\top$, and make the change of variable $\mathbf{y} = A\mathbf{x}$, so that

$$\mathbf{y}^\top \Sigma^{-1} \mathbf{y} = \mathbf{x}^\top \mathbf{x}.$$

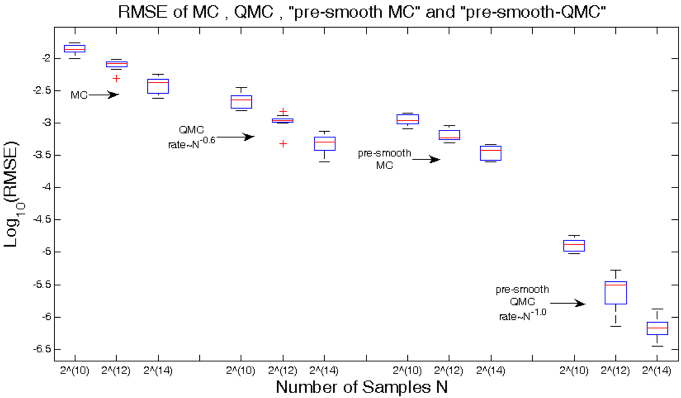
Specifically we make the PCA choice for $A$, i.e.

$$A = \left[ \sqrt{\lambda_1}\eta_1, \ldots, \sqrt{\lambda_d}\eta_d \right],$$

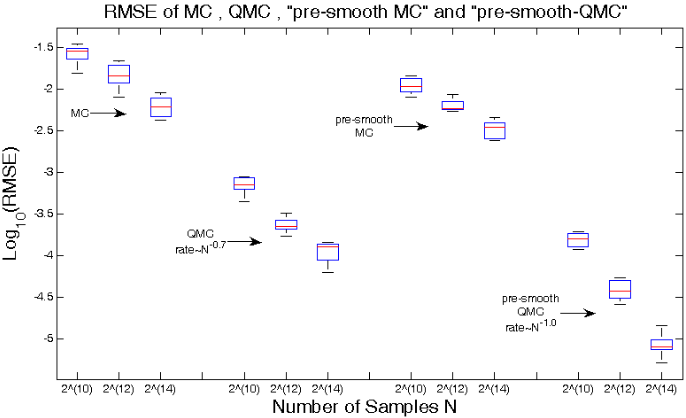
where $\lambda_1, \ldots, \lambda_d$ are eigenvalues of $\Sigma$ in decreasing order, and $\eta_1, \ldots, \eta_d$ are the corresponding eigenvectors.



RMSE of MC , QMC , "pre-smooth MC" and "pre-smooth-QMC"
Log10(RMSE)
-1.5
-2
-2.5
-3
-3.5
-4
-4.5
-5
-5.5
-6
MC
QMC
rate~N^-1.0
pre-smooth
MC
pre-smooth
QMC
rate~N^-1.0
2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14)
Number of Samples N


RMSE of MC , QMC , "pre-smooth MC" and "pre-smooth-QMC"
Log10(RMSE)
-2
-2.5
-3
-3.5
-4
-4.5
-5
-5.5
-6
-6.5
MC
QMC
rate~N^-0.6
pre-smooth
MC
pre-smooth
QMC
rate~N^-1.0
2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14) 2^(10) 2^(12) 2^(14)
Number of Samples N

# Asian Option Brownian Bridge



# Conclusion and Outlook

- Smooth simple kinks or jumps in one variable can be eliminated by preintegration operator $P_\psi$.
- Varience is reduced by Sobol Index, yielding benefits for MC and QMC
- $P_\psi$ maintains Differentiability and (mathematical) Integrability under certain (strong) assumptions .
- Boundedness of $P_\psi$ remains to be shown in suitable functional setting.
- In principle nested preintegration possible in presence of intersecting kinks and jumps.

# Path Integral Quantization of the An- & Harmonic Oscillator

class. eucl. Action: $S = \int dt \left[ \frac{M}{2} \dot{x}(t)^2 + V(x(t)) \right]$

P.I. quantization: $Z = \int \mathcal{D}[x(t)] e^{-S[x,\dot{x}]}$

harmonic Oscillator: $V(x) = \frac{\mu^2}{2} x^2 \; ; \quad \mu^2 > 0$

anharmonic Oscillator: $V(x) = \frac{\mu^2}{2} x^2 + \lambda x^4 \; ; \quad \mu^2 \in \mathbb{R}, \; \lambda > 0$

# Structure of the action

generally the lattice action can be written in the form

$$S = \frac{1}{2} x^t C^{-1} x + a\lambda \sum_{i=1}^{d} x_i^4$$

$$C^{-1} = \frac{2M}{a} \begin{pmatrix} u & -\frac{1}{2} & 0 & \dots & 0 & -\frac{1}{2} \\ -\frac{1}{2} & \ddots & \ddots & \ddots & \vdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & \ddots & \ddots & -\frac{1}{2} \\ -\frac{1}{2} & 0 & \dots & 0 & -\frac{1}{2} & u \end{pmatrix}$$

$$u = 1 + \frac{a^2 \mu^2}{2M} \tag{3}$$

- $C$ is covariance matrix of the variables $x_i$ if $\lambda = 0$

observable of the harmonic oscillator:

$$\langle O \rangle = \frac{\int \ O(x)\ e^{-\frac{1}{2}x^T C^{-1} x} d\mathbf{x}}{\int \ e^{-\frac{1}{2}x^T C^{-1} x} d\mathbf{x}} \overset{(C=C_{sim})}{=} \frac{I(O(x))}{I(1)}$$

observable of the anharmonic oscillator:

$$\langle O \rangle = \frac{\int \ O(x)\ e^{-\frac{1}{2}x^T C^{-1} x - a \sum_i x_i^4} d\mathbf{x}}{\int \ e^{-\frac{1}{2}x^T C^{-1} x - a \sum_i x_i^4} d\mathbf{x}} = \frac{I(O(x)W(x))}{I(W(x))} \tag{4}$$

$$W(\mathbf{x}) = \exp -\frac{1}{2}\mathbf{x}^t (C^{-1} - C_{sim}^{-1})\mathbf{x} - a \sum_i x_i^4 \tag{5}$$

( $C_{sim} \neq C$ because if $\mu^2 < 0 \Rightarrow C_{sim} \not> 0$)

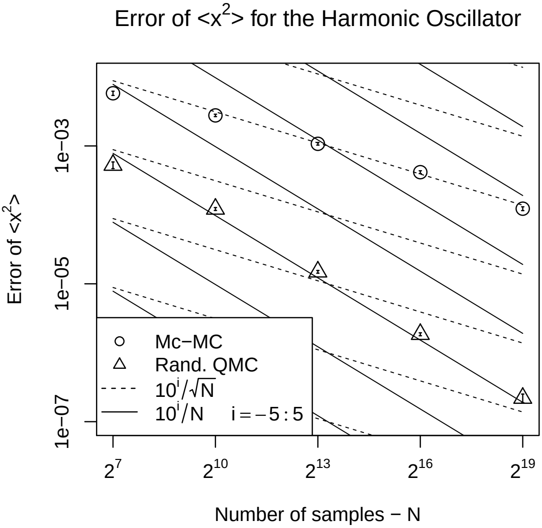
# Observables

- $X^2 = \frac{1}{d}\sum_{i=1}^{d} x_i^2$
- $X^4 = \frac{1}{d}\sum_{i=1}^{d} x_i^4$
- $E_0 = \mu^2 X^2 + 3\lambda X^4 + \frac{\mu^4}{16}$
- Correlator: $C(t) = \frac{1}{d}\sum_{i=1}^{d} x_i x_{i+t/a}$ (not implemented so far)

Parameters:

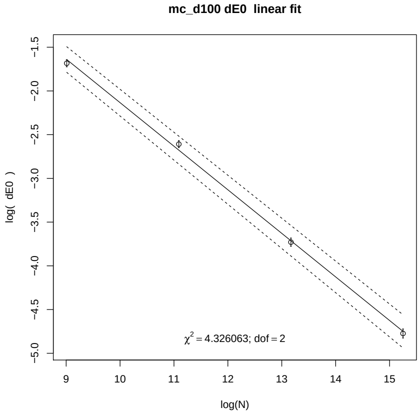
- $\rightarrow$ Blackboard

# Warm-up Exercise: Harmonic Oscillator




- trivial, but we demonstrated applicability to physical problems
- **three digits** more accuracy with QMC at $N = 5 \times 10^5$

# Anharmonic Oscillator, MC points, $O = E_0$, $d = 100$

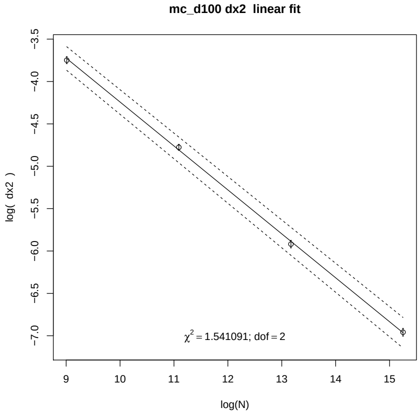



Fit formula:

$$\log \Delta(E_0) = \log C + \alpha \log N$$

- $\alpha = -0.50(1)$
- $\log C = 2.84(12)$

# Anharmonic Oscillator, MC points, $O = X^2$, $d = 100$

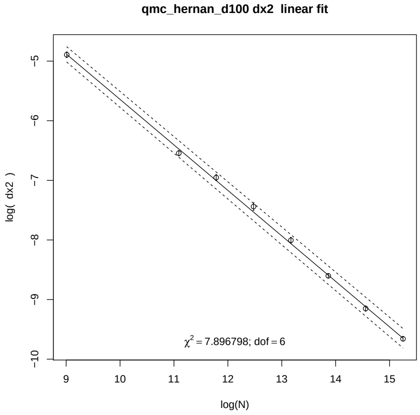



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.52(1)$
- $\log C = 0.94(11)$

# Anharmonic Oscillator, QMC points, $O = X^2$, $d = 100$

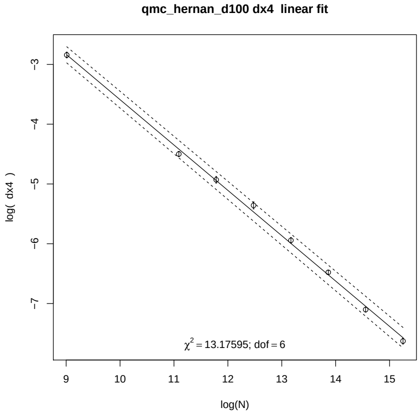



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.76(1)$
- $\log C = 2.0(1)$

# Anharmonic Oscillator, QMC points, $O = X^4$, $d = 100$

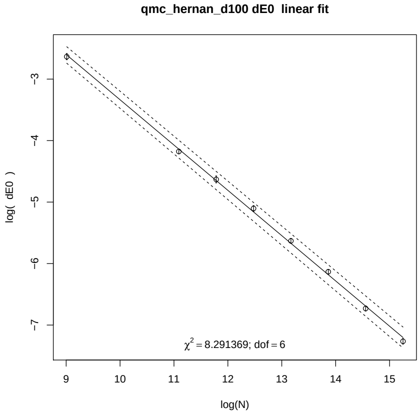



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.76(1)$
- $\log C = 4.0(1)$

# Anharmonic Oscillator, QMC points, $O = E_0$, $d = 100$

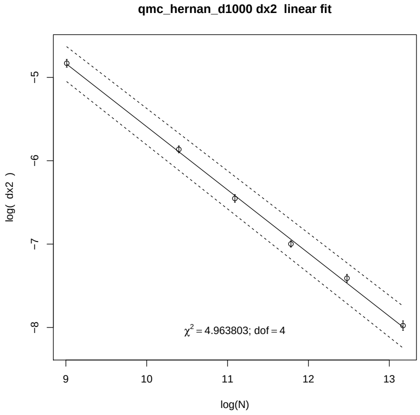



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = 0.74(1)$
- $\log C = 4.0(1)$

# Anharmonic Oscillator, QMC points, $O = X^2$, $d = 1000$

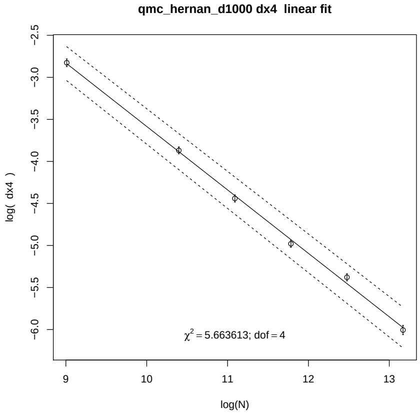



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.76(1)$
- $\log C = 2.0(2)$

# Anharmonic Oscillator, QMC points, $O = X^4$, $d = 1000$

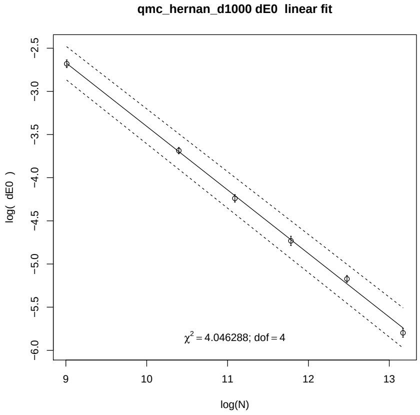



Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.75(1)$
- $\log C = 4.0(2)$

# Anharmonic Oscillator, QMC points, $O = E_0$, $d = 1000$




Fit formula:

$$\log \Delta(X^2) = \log C + \alpha \log N$$

- $\alpha = -0.74(1)$
- $\log C = 4.0(2)$