Recursive Numerical Integration

Improve error scaling of lattice simulations

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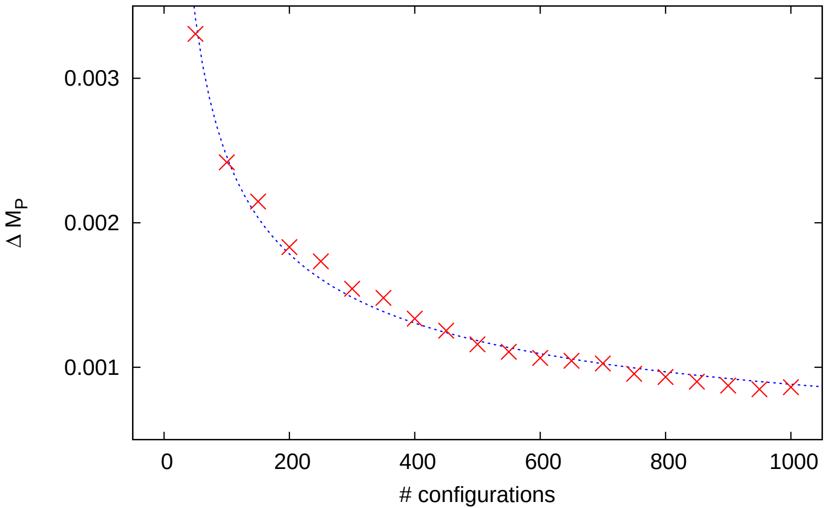
DESY Zeuthen

26. Juli 2016

Problems of Markov Chain Monte Carlo (MCMC)



$$\Delta M_P \sim \frac{1}{\sqrt{\#\text{configurations}}}$$

Recursive Numerical Integration

[Genz, Kahaner 1986] [Hayter 2005]

Recursive Numerical Integration

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$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x\, O[x]\, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x\; \mathrm{e}^{-S[x]}} = \frac{A}{B}$$

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$$B = \mathrm{Tr}[M^d]$$

$$A(O) = \sum \mathrm{Tr}[A_1 A_2 \ldots A_d]$$

Recursive Numerical Integration

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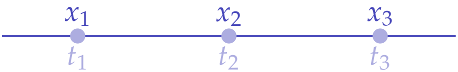
Recipe

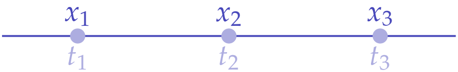
1. Split Integral
2. Numerical Integration
3. Reduction to Linear Algebra

- **Split Integral**



$$x_i \in [-\pi, \pi)$$

• Split Integral



$x_i \in [-\pi, \pi)$

$$B = \int_{[-\pi,\pi]^3} \mathrm{d}x \;\; \exp\left(-S[x]\right)$$

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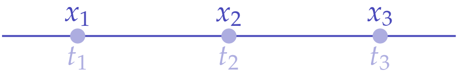

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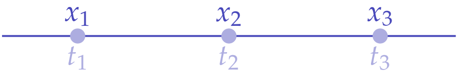
$$= \int_{[-\pi,\pi]^3} \mathrm{d}x \;\; \exp\left(-\sum_{i=1}^{3} S\left(x_{i+1}, x_i\right)\right)$$

NN coupling

• Split Integral



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$$
\begin{aligned}
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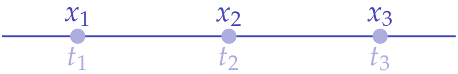
&= \int_{[-\pi,\pi]^3} \mathrm{d}x \;\; \prod_{i=1}^{3} \exp\left(-S(x_{i+1}, x_i)\right)
\end{aligned}
$$

NN coupling

• Split Integral



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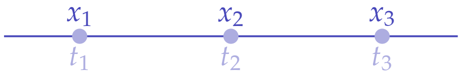

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&= \int_{[-\pi,\pi]^3} \mathrm{d}x \;\; \prod_{i=1}^{3} \underbrace{\exp\left(-S(x_{i+1}, x_i)\right)}_{f(x_{i+1}, x_i)} \\
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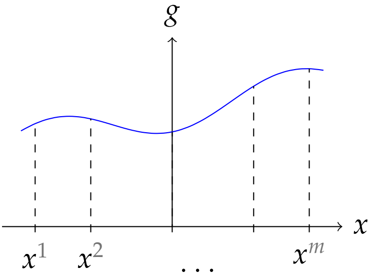
\end{aligned}
$$

• Numerical Integration & • Lin. Algebra

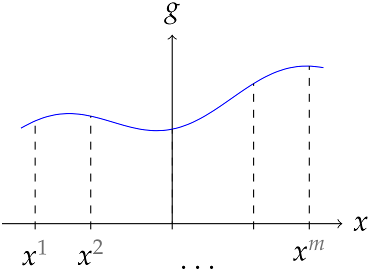


Gauss

$$\int_{-1}^{1} \mathrm{d}x\, g(x) = \sum_{r=1}^{m} w^r g(x^r) + \mathcal{O}\left(\frac{1}{(2m)!}\right)$$

$$g(x) \approx P_{2m-1} = \sum_{i=0}^{2m-1} a_i x^i$$

• Numerical Integration & • Lin. Algebra



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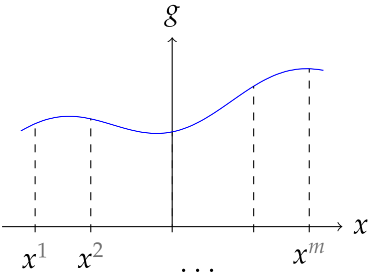
x^r, w^r : $L_m(x)$ Legendre polynoms

• Numerical Integration & • Lin. Algebra



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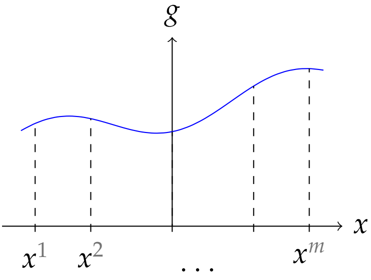
• Numerical Integration & • Lin. Algebra



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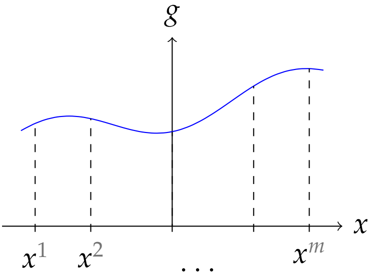

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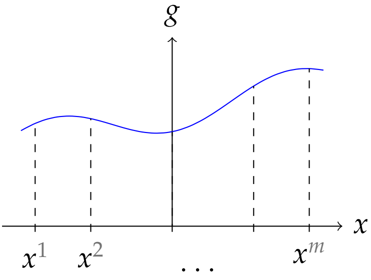

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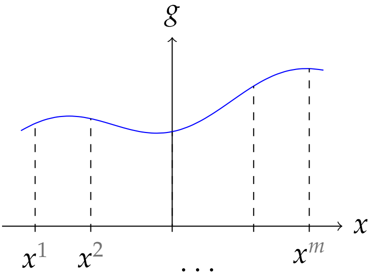
• Numerical Integration & • Lin. Algebra



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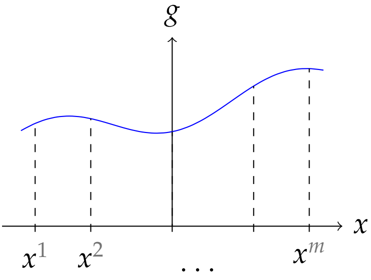

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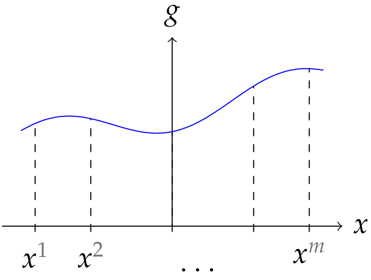

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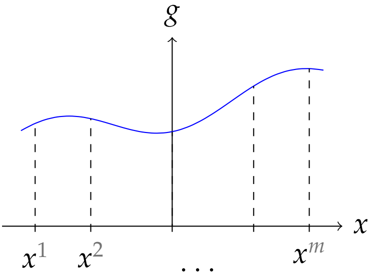
• Numerical Integration & • Lin. Algebra



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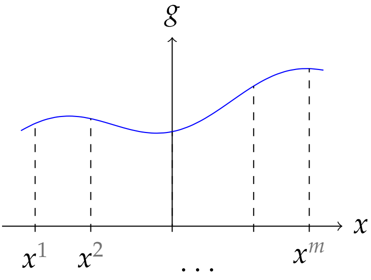
• Numerical Integration & • Lin. Algebra



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$$= \mathrm{Tr}[M^3] = \sum_i \lambda_i^3$$

$M \in \mathbb{R}^{m\times m}, m = 500$ suffies

More General

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x \, O[x] \, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x \; \mathrm{e}^{-S[x]}} = \frac{A}{B}$$

$$\begin{aligned} B &= \int_{-\pi}^{\pi} \mathrm{d}x_1 \int_{-\pi}^{\pi} \mathrm{d}x_2 \; f(x_2, x_1) \cdot \int_{-\pi}^{\pi} \mathrm{d}x_3 \; f(x_3, x_2) \cdot f(x_1, x_3) \\ &= \mathrm{Tr}[M^3] \to \mathrm{Tr}[M^d] \end{aligned}$$

$$A(O) = ... \to \sum \mathrm{Tr}[\; A_1 A_2 \ldots . A_d]$$

More General

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x\, O[x]\, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x\ \mathrm{e}^{-S[x]}} = \frac{A}{B}$$

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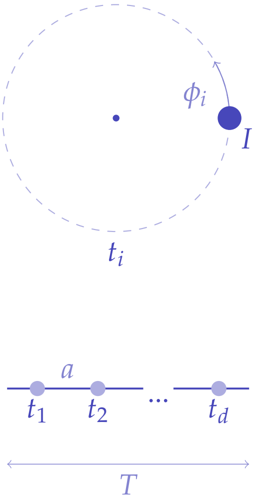
$$= \mathrm{Tr}[M^3] \to \mathrm{Tr}[M^d]$$

$$A(O) = ... \to \sum \mathrm{Tr}[\ \underbrace{A_1 A_2 \ldots}_{\text{e.g. } (A_1)^k, k<d}\ . A_d]$$

Topological Oscillator



$$S(\phi) = \int_0^T \mathrm{d}t \, \frac{I}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 \qquad \phi \in [-\pi, \pi)$$

$$\rightarrow \frac{I}{a} \sum_{i=1}^{d} (1 - \cos(\phi_{i+1} - \phi_i))$$

Topological Charge

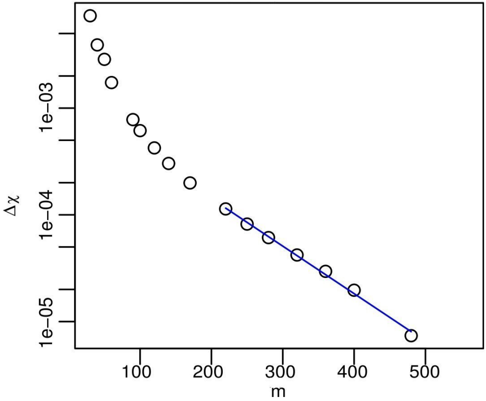
$$Q(\phi) = \frac{1}{2\pi} \int_0^T \mathrm{d}t \, \left(\frac{\partial \phi}{\partial t} \right) \in \mathbb{Z}$$

$$\rightarrow \frac{1}{2\pi} \sum_{i=1}^{d} (\phi_{i+1} - \phi_i) \mod [-\pi, \pi)$$

Topological Susceptibility

$$\chi = \frac{\langle Q^2(\phi) \rangle}{T}$$

Truncation Error Scaling



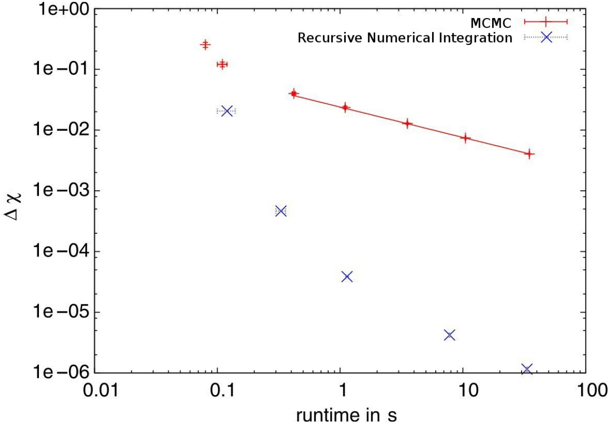
$\propto e^{-c \cdot m}$

Error $\Delta\chi_i = |\chi_i - \chi(m = 560)|$

Constants $I = 0.25$

$a = 0.4, T = 20$

Comparison with MCMC



$\propto \frac{1}{\sqrt{t}}$

Error $\Delta\chi_{i,Gauss} = |\chi_i - \chi(m = 400)|$

$\Delta\chi_{i,Cluster}$: 10 runs

Constants $I = 0.25$

$a = 0.1, T = 20$

Conclusion [arXiv: 1503.05088]

Goal

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x\, O[x]\, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x\, \mathrm{e}^{-S[x]}} = \frac{A}{B}$$

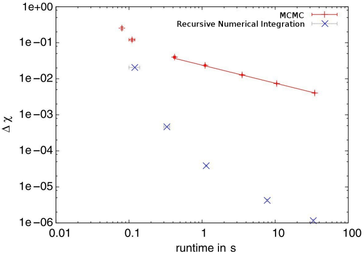
Method Recursive Numerical Integration

$$B = \int_{D^d} \mathrm{d}x \ \prod_{i=1}^{d} \exp\left(-S(x_{i+1}, x_i)\right) = \mathrm{Tr}[M^d]$$

$$A = \sum \mathrm{Tr}[A_1 A_2 \ldots A_d] \qquad M \in \mathbb{R}^{500\times 500} \text{ suffies}$$

Results Topological Oscillator

Anharmonic Oscillator



Problems higher dimensions

Future other methods [T. Hartung, Mo 18:05]

How to calculate A

$$\langle O \rangle = \frac{\int_{D^d} \mathrm{d}x \, O[x] \, \mathrm{e}^{-S[x]}}{\int_{D^d} \mathrm{d}x \; \mathrm{e}^{-S[x]}} = \frac{A}{B}$$

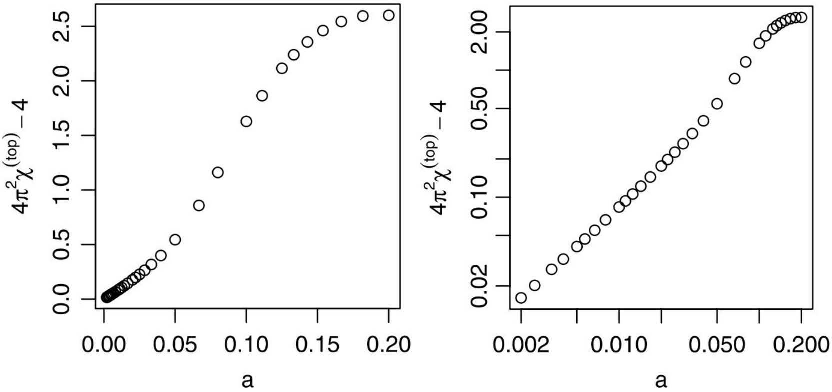
$$B = \int_{-\pi}^{\pi} \mathrm{d}x_1 \int_{-\pi}^{\pi} \mathrm{d}x_2 \; f(x_2, x_1) \cdot \int_{-\pi}^{\pi} \mathrm{d}x_3 \; f(x_3, x_2) \cdot f(x_1, x_3) = \mathrm{Tr}[M^3]$$

$$O[x] = (x_1^2 + x_2^2 + x_3^2)$$

$$\begin{aligned} A = &\Bigg(\int_{-\pi}^{\pi} \mathrm{d}x_1 \, x_1^2 \int_{-\pi}^{\pi} \mathrm{d}x_2 \; f(x_2, x_1) \cdot \int_{-\pi}^{\pi} \mathrm{d}x_3 \; f(x_3, x_2) \cdot f(x_1, x_3) \\ &+ \int_{-\pi}^{\pi} \mathrm{d}x_1 \int_{-\pi}^{\pi} \mathrm{d}x_2 \, x_2^2 \, f(x_2, x_1) \cdot \int_{-\pi}^{\pi} \mathrm{d}x_3 \; f(x_3, x_2) \cdot f(x_1, x_3) \\ &+ \int_{-\pi}^{\pi} \mathrm{d}x_1 \int_{-\pi}^{\pi} \mathrm{d}x_2 \; f(x_2, x_1) \cdot \int_{-\pi}^{\pi} \mathrm{d}x_3 \, x_3^2 \, f(x_3, x_2) \cdot f(x_1, x_3) \Bigg) \\ &= \sum_{i=1}^{3} \mathrm{Tr}[M A_i M] \end{aligned}$$

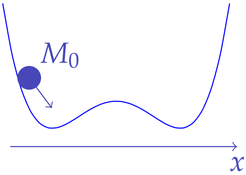
Topological Oscillator - χ in the continuum

$$\chi_{theo} \to \frac{1}{4\pi^2 I} \qquad I = 0.25 = const, \qquad m = 120, \qquad d = \frac{20}{a}$$



(a) linear (b) logarithmic

Anharmonic Oscillator



$$S(\phi) = \frac{M_0}{2}\left(\frac{\partial x}{\partial t}\right)^2 + \frac{\mu^2}{2}x^2 + \lambda x^4,\ x \in (-\infty, \infty)$$

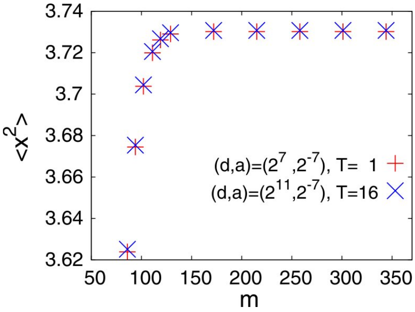
$$\to a \sum_{i=0}^{d-1}\left[\frac{M_0}{2a^2}(x_{i+1} - x_i)^2 + \frac{\mu^2}{2}x_i^2 + \lambda x_i^4\right]$$

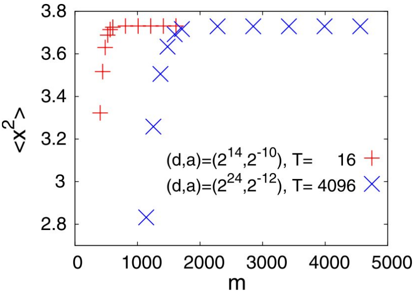
Powers of Particle Position

$$\langle x^2 \rangle = \frac{1}{d}\sum_{i=0}^{d-1} x_i^2$$

Anharmonic Oscillator Observable: $\langle x^2 \rangle$

$x \in (-\infty, \infty) \rightarrow x \in (-l, l), l > 0$ such that $\langle x^2 \rangle_{\text{cut}} / \langle x^2 \rangle < 10^{-10}$





- $\lambda = 1.0, M_0 = 0.5, \mu^2 = -16.0$
- $T = 4096$: $t < 3$ min

$$E_0 = \mu^2 \langle x^2 \rangle + 3\lambda \langle x^4 \rangle + \frac{\mu^2}{16} : E_{0,T=4096} = 3.86367053759882$$

$$E_{0,\text{exact}} = 3.8636669$$