Mitigating the sign problem with line integrals

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What is the sign problem

- We wish to solve integrals like

$$< O > \quad = \quad \frac{\int d^N x O(x) \exp(-E(x))}{\int d^N x \exp(-E(x))} \tag{1}$$

- Monte-Carlo methods can solve this by sampling with probability $\rho(x) = \exp(-E(x))$
- Precision of Monte-Carlo goes like $1/\sqrt{measurements}$
- If E is complex we cannot use it as a probability distribution anymore

What is the sign problem 2

- One can instead try to sample on the real part of E(x)

$$< O > \;=\; \frac{\int d^N x O(x) \frac{\exp(-E(x))}{|\exp(-E(x))|} |\exp(-E(x))|}{\int d^N x \frac{\exp(-E(x))}{|\exp(-E(x))|} |\exp(-E(x))|} \qquad (2)$$

- One then have to measure $O(x)\frac{\exp(-E(x))}{|\exp(-E(x))|}$ and $\frac{\exp(-E(x))}{|\exp(-E(x))|}$ and take the ratio.
- Second measurement often called the average phase (for short I write $< 1 >$)
- If imaginary part of E changes quickly, the integral will flip between $+$ and $-$ often, such that $< 1 >$ becomes small
- Precision of Monte-Carlo goes like $1/\sqrt{measurements}$
- If $< 1 >= 10^{-5}$ then we need atleast 10^{10} extra measurements

Motivation

- Reduce the sign problem
- Some systems can be well approximated by expanding around the stable points
  - Airy functions $\int_{-\infty}^{\infty} \cos(t^3/3 + tx)dt$ behavior of oscilating or exponential damped can be explained by whether the stable point is real or complex
- Does not want to calculate the determinant or products of non-sparse matrices
  - Continuation into the complex plane requires one to calculate a determinant that cost (lattice size $)^3$
- Does not require analytic continuation
  - Would like to be able to simulate systems like a coulomb potential which have poles
- Sample along regions of importance
  - Methods like density of state measures a lot of unimportant regions, only for them to cancel in post-production

Motivation 2

- Attempted solution:
  - Change sampling from a point to a line
- Many possible lines:
  - Follow lines where the imaginary part of the action is changing, such that oscillations will cancel out

Overview

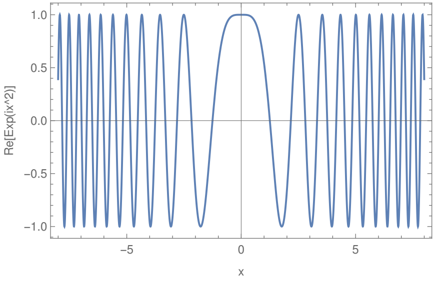
- The path of the lines
- Sampling lines with equal probability
- The line Integral
- Cutoff on integral region
- Implementation
  - Usage example: 1D Quantum mechanical Anharmonic oscillator with x^4 potential
- https://arxiv.org/pdf/2205.02257.pdf

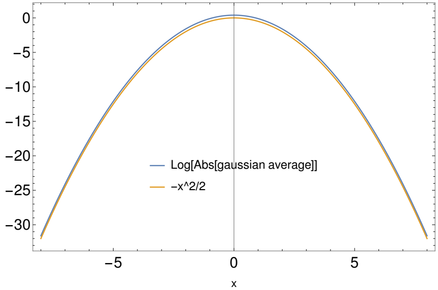
The path of the lines

- Will focus on systems that can be written as

$$\langle O \rangle = \int d^N x \exp(-E(x)) \frac{O(x)}{Z}, \quad E \in \mathbb{C} \tag{3}$$

- Want to sample lines from which oscillations will cancel
- Behavior of $Re[\exp(ix^2)]$ shown below



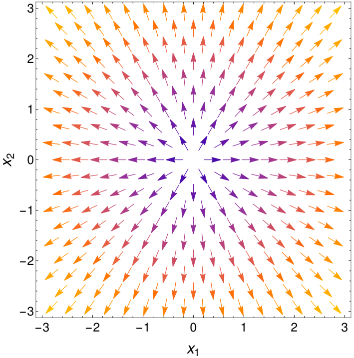


Example

- In dimension higher than 1, there is only one direction locally where the imaginary part if changing
- Solution: Follow the direction in which the imaginary part of the Energy or action E (depending on the system of interest) changes

$$\frac{\partial E_{im}(x)}{\partial x_j} \equiv F_j(x)$$
$$\frac{dx_j}{d\tau} = F_j(x)$$

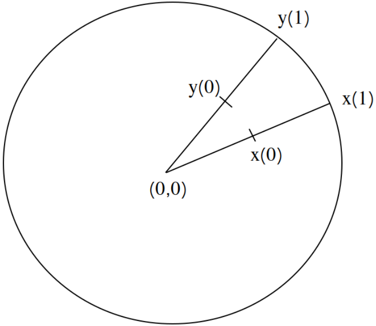
- Example on the right: $E = i(x_1^2 + x_2^2)$



Sampling lines with equal probability

- We need to make sure that every point is counted the same amount of times
- Include volume factor V_{rel} for how often a point is counted, compared to start position of line

- Example: $E = i(x_1^2 + x_2^2)$
- 2 Slightly different starting points $x(0)$ and $y(0)$
- At later time (1) the points are further separated
- Need to count contribution to line integral as $\left|\frac{x(1)}{x(0)}\right|$
- Similar to radial coordinates



Change in volume factor

- We look at the change of the unit vectors v under a infinitesimal change with the force

$$
\begin{aligned}
\left[dx_i(x+\epsilon_2 v) - dx_i(x)\right]/\epsilon_2 &= \\
\epsilon\left[F_i(x+\epsilon_2 v) - F_i(x)\right]/\epsilon_2 &= \epsilon\frac{\partial^2 E_{im}(x)}{\partial x_i \partial x_j} v_j + O(\epsilon_2) \\
\frac{V_{rel}(\tau+\epsilon)}{V_{rel}(\tau)} = \det\left[I_{ij} + \epsilon\frac{\partial^2 E_{im}(x(\tau))}{\partial x_i \partial x_j}\right] &= 1 + \epsilon\sum_{j=1}^{N}\frac{\partial^2 E_{im}(x(\tau))}{\partial^2 x_j} \\
&\quad + O(\epsilon^2)
\end{aligned} \tag{4}
$$

- The change of the volume factor is therefore proportional to the size of the lattice

$$
\frac{d\log(V_{rel}(\tau))}{d\tau} = \sum_{j=1}^{N}\frac{\partial^2 E_{im}(x(\tau))}{\partial^2 x_j} \tag{5}
$$

The line integral

- Collecting everything into an integral gives us

$$I_O(x_0) = \int_{-\infty}^{\infty} O(x(s)) \exp\left[-E(x(s))\right] V_{rel}(s) ds \quad (6)$$
$$= \int_{-\infty}^{\infty} O(x(\tau)) \exp\left[-E(x(\tau)) + \sum_{j=1}^{N} \int_0^{\tau} \frac{\partial^2 E_{im}(x(\tau'))}{\partial^2 x_j} d\tau'\right] |F(x_0)| d\tau$$

- $x(\tau)$ is obtained by following the defined path in both positive and negative τ
- s is the distance traveled along the line

$$\frac{ds}{d\tau} = |F(x(\tau))| \quad (7)$$

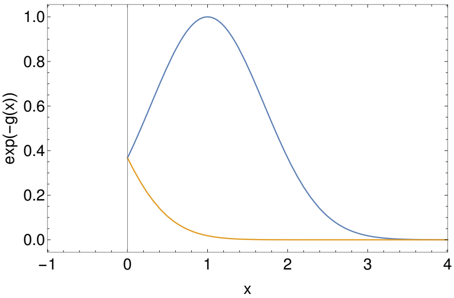
Cutoff the line integral

- We do not want to sample all the way out to infinity
- Cutoff integral with small trick

$$\int_{-\infty}^{\infty} \exp(-E(x))dx = \text{constant} \cdot \int_{-\infty}^{\infty} \exp(-\mathrm{E}(\mathrm{x}) - \mathrm{g}(\mathrm{s}))\mathrm{dxds} \quad (8)$$

$$= \text{constant} \cdot \int_{-\infty}^{\infty} \exp(-\mathrm{E}(\mathrm{x}+\mathrm{s}) - \mathrm{g}(\mathrm{s}))\mathrm{dxds} \quad (9)$$

- Example with $g(s) = s^2$, starting at $x = 1$
- In case a stable point is hit, direction of integration should be reversed, but s should keep increasing



Implementation

- The entire procedure can be implemented as a set of differential equations

$$F_j(x) = \frac{\partial E_{im}}{\partial x_j} = \frac{dx_j}{d\tau} \quad (10)$$

$$\frac{ds}{d\tau} = \sqrt{\sum_{j=1}^{N} F_j(x)^2} \quad (11)$$

$$\frac{dJ}{d\tau} = \sum_{j=1}^{N} \frac{\partial^2 E_{im}}{\partial^2 x_j} \quad (12)$$

$$\frac{dI_O}{d\tau} = O(x(\tau))e^{-E(x(\tau))-g(s)+J}|F(x_0)| \quad (13)$$

$$I_O = I_O(\tau = \infty) - I_O(\tau = -\infty) \quad (14)$$

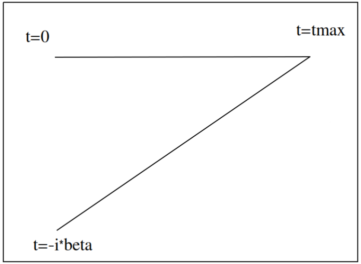
- We have defined $J = \log(V_{rel}(\tau))$
- $|F(x_0)|$ can be absorbed into the initial conditions of J
- [illegible]

Example: 1d anharmonic oscillator

- As an example of its usage we calculate the correlator for

$$
\begin{aligned}
< O > &= Tr(e^{-\beta H} x e^{-itH} x e^{itH}) / Tr(e^{-\beta H}) \quad (15) \\
H &= \frac{p^2}{2} + \frac{x^2}{2} + \frac{\lambda x^4}{4!} \quad (16)
\end{aligned}
$$

- Write system as path integral along a schwinger keldysh path
- We will look at the strongly coupled case $\lambda = 24$
- $\beta = 1.0$
- Compare with solution from discretizing x



Approach

- The derivatives needed to calculate the lines becomes

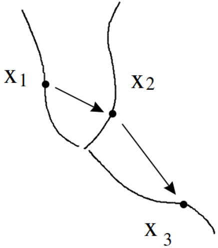
$$
\begin{aligned}
\langle O \rangle &= \int d^N x \exp\left(\sum_{j=1}^{N} i[\frac{(x_j - x_{j+1})^2}{2a_j} - \frac{(a_j + a_{j-1})}{2}(\frac{x_j^2}{2} + \frac{\lambda x_j^4}{4!})] \right) \frac{O(x)}{Z} \\
E &= -\sum_{j=1}^{N} i[\frac{(x_j - x_{j+1})^2}{2a_j} - \frac{(a_j + a_{j-1})}{2}(\frac{x_j^2}{2} + \frac{\lambda x_j^4}{4!})] \\
\frac{\partial E_{im}}{\partial x_j} &= -Im \left(i[\frac{(x_j - x_{j+1})}{a_j} + \frac{(x_j - x_{j-1})}{a_{j-1}} - \frac{(a_j + a_{j-1})}{2}(x_j + \frac{\lambda x_j^3}{3!})] \right) \\
\frac{\partial^2 E_{im}}{\partial^2 x_j} &= -Im \left(i[\frac{1}{a_j} + \frac{1}{a_{j-1}} - \frac{(a_j + a_{j-1})}{2}(1 + \frac{\lambda x_j^2}{2})] \right)
\end{aligned}
$$

Importance Sampling

$$\langle O \rangle = \frac{\int d^N x I_O(x)}{\int d^N x I_1(x)} = \frac{\int d^N x |I_1(x)| \times I_O(x)/|I_1(x)|}{\int d^N x |I_1(x)| \times I_1(x)/|I_1(x)|} \tag{17}$$

- We will sample on the start position of the line using the metropolis algorithm

$$\langle O \rangle = \frac{\sum_j I_O(x_j)/|I_1(x_j)|}{\sum_j I_1(x_j)/|I_1(x_j)|}$$
$$O = x(0)x(t)$$

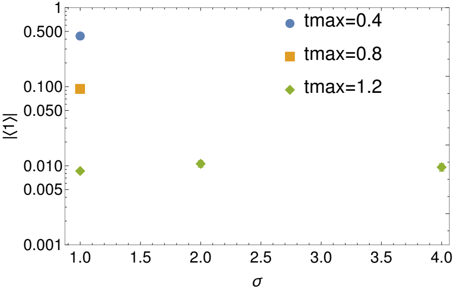


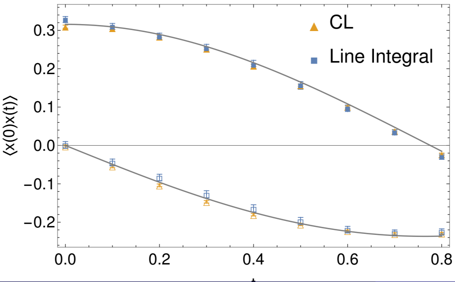
- The subscript O indicates the observable included in the line integral and j indicates the j'th measurement
- We define the average phase $\langle 1 \rangle$ as

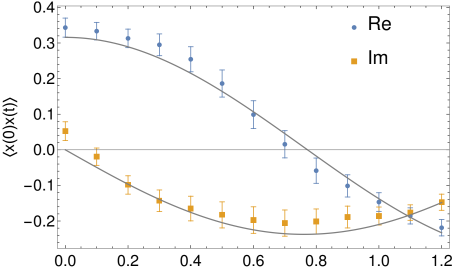
$$\langle 1 \rangle = \frac{1}{N_{sampl}} \sum I_1(x_j)/|I_1(x_j)| \tag{18}$$

Correlator

- $\langle x(0)x(t)\rangle$
- Correlator is possible up around $t = 1.2$
- Average sign becomes too small afterwards







Summary

- We have defined a set of line integrals whose sum adds up to the original integral
- The lines are defined such that oscillations cancels out
- The lines can be implemented using standard ordinary differential equations

- Shown example of strongly coupled anharmonic oscilator
- Cost due to average sign and other hidden cost like precision limits us currently to $t_{max} = 1.2$
- Still room for optimization