# Density of observables from local derivatives

Rasmus N. Larsen

University of Bielefeld

August 2. 2024

Talk based on Paper: https://arxiv.org/pdf/2401.01211
Work done at the University of Stavanger

# Motivation

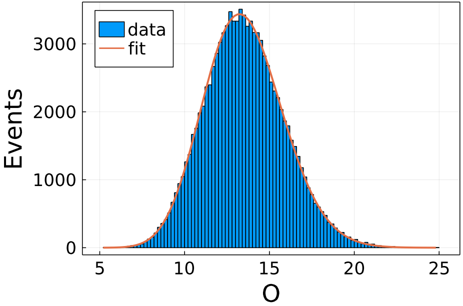
- Improve precision of lattice measurements by using smooth behavior of observable $O$ and action $S$

$$\langle f(O) \rangle = \frac{\int d^D x f(O(x)) \exp(-S(x))}{\int d^D x \exp(-S(x))} \quad (1)$$

- Precision from random sampling from Monte-Carlo methods scale as $1/\sqrt{\#Samples}$

$$\langle f(O) \rangle = \frac{\int dO f(O)\rho(O)}{\int dO \rho(O)} \quad (2)$$

- If one looks at the density of state for an observable $\rho(O)$, quite large fluctuations are observed even at high statistics
- Improvements to the precision of the density of state has been done in the LLR method, where the slope at many values of O are sampled, to make a smoother density
- Fit shows results from the technique I will discuss



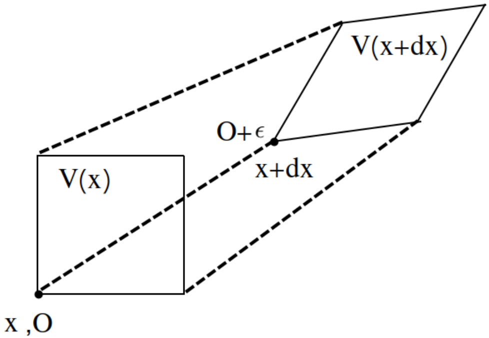
# Attempted solution

- Observation:
  - In a D dimensional space a vector, like $\frac{\partial O(x)}{\partial x_j} \equiv O_j(x)$ is orthogonal to $D-1$ other vectors, such that we only have to worry about the change to O along this direction
  - The density of state is a measure of how large the volume, scaled by $\exp(-S)$, is for a value of the observable O
- Attempted Solution:
  - Look at how the volume changes from one value of $O$, to another value $O+\epsilon$

$$\frac{1}{\epsilon}\log(V(O+\epsilon)/V(O)) \quad = \quad \frac{1}{\epsilon}\log(\rho(O+\epsilon)/\rho(O)) = \frac{d\log(\rho(O))}{dO} + R(\epsilon)$$

- $dx_i = \epsilon\frac{O_i}{O_j^2}$, sum when index appears twice, square included
- The change to the relative local volume along a direction can be calculated as [arxiv:2205.02257]

$$dV(x) \quad \equiv \quad \partial_{x_i}(\frac{O_i}{O_j^2}) = \frac{O_{i,i}}{O_j^2} - \frac{2O_iO_{i,j}O_j}{(O_k^2)^2}$$



# Average change

- We look for how the total volume changes from $O$ to $O + \epsilon$
- We assume that each $O(x)$ was sampled in a Monte-Carlo sampling of $\exp(-S)$

$$\begin{aligned}
V(O+\epsilon) &= V_{norm}(\sum_{O(x)=O} \exp[\epsilon dV - (S(x_i + dx_i) - S(x_i))]) \\
&= V_{norm} N_{samples}(1 + \epsilon(\langle dV \rangle - \langle \frac{S_i O_i}{O_j^2} \rangle) + R(\epsilon^2)) \quad (3) \\
\log[V(O+\epsilon)/V(O)] &= \log[1 + \epsilon(\langle dV \rangle - \langle \frac{S_i O_i}{O_j^2} \rangle)] + R(\epsilon^2))) \quad (4) \\
&= \epsilon(\langle dV \rangle - \langle \frac{S_i O_i}{O_j^2} \rangle) + R(\epsilon^2) \\
d_O \log(\rho(O)) &= \langle dV \rangle - \langle \frac{S_i O_i}{O_j^2} \rangle \quad (5) \\
&= \langle \frac{O_{i,i}}{O_j^2} - \frac{2 O_i O_{i,j} O_j}{(O_k^2)^2} - \frac{S_i O_i}{O_j^2} \rangle \quad (6)
\end{aligned}$$

- Average is for all x where $O(x) = O$

# Simple Example

- $S = O = x_i^2$
- $\langle O \rangle = \frac{1}{Z} \int x_i^2 \exp(-x_j^2) d^D x$

$$d_O \log(\rho(O)) = \langle \frac{O_{i,i}}{O_j^2} - \frac{2O_i O_{i,j} O_j}{(O_k^2)^2} - \frac{S_i O_i}{O_j^2} \rangle \quad (7)$$

$$O_i = \partial_{x_i}(x_j^2) = 2x_i \quad (8)$$

$$O_{i,i} = \partial_{x_i}^2(x_j^2) = 2D \quad (9)$$

$$O_i^2 = 4x_i^2 = 4S \quad (10)$$

$$O_i O_{i,j} O_j = 2x_i 2\delta_{i,j} 2x_j = 8x_i^2 = 8S \quad (11)$$

$$d_S \log(\rho(S)) = \frac{2D}{4S} - \frac{2 * 8S}{(4S)^2} - 1 = \frac{1}{S}(D/2 - 1) - 1 \quad (12)$$

- The last differential equation can then be solved which gives

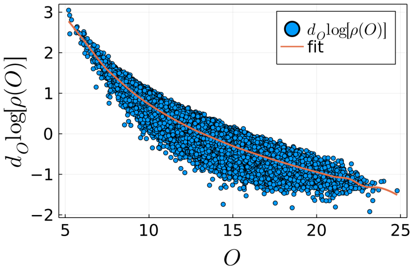
$$\rho(S) = Constant * \exp(\log(S)(D/2 - 1) - S) = Constant * S^{D/2-1} \exp(-S)$$

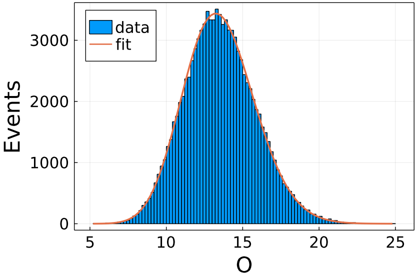
# Less Simple Example

- $S = x_j^4$
- $O = x_j^2$
- $D = 40$
- Fitted with spline of order 25

| N | Observable | Re | Im |
|---|---|---|---|
| $10^5$ | O | $13.515 \pm 0.018$ | 0 |
| $10^6$ | O | $13.512 \pm 0.005$ | 0 |
| $10^7$ | O | $13.521 \pm 0.001$ | 0 |
| $10^5$ | dV | $13.523 \pm 0.007$ | 0 |

Table: Exact result is $13.5196$.



# SU3

- Changes to SU3 is done by the 8 generators $\tau_i$ of the su3 algebra

$$U \to \exp(i\epsilon_j \tau_j)U \tag{13}$$

- We find that there is no change to the volume of the group elements from this change, since the metric is trivial under this transformation [Jan Smith, Introduction to Quantum Fields on a Lattice]

$$2tr\left(\frac{\partial U}{\partial \alpha_k}\frac{\partial U^\dagger}{\partial \alpha_l}\right) \quad = \quad 2tr[(i\tau_k)U(i\tau_l U)^\dagger] = 2tr(\tau_k\tau_l) = 4\delta_{k,l} \tag{14}$$

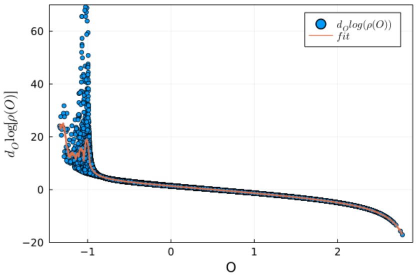
- The volume around each point in SU3 for left multiplication is therefore constant, and the derived formula will therefore still work.

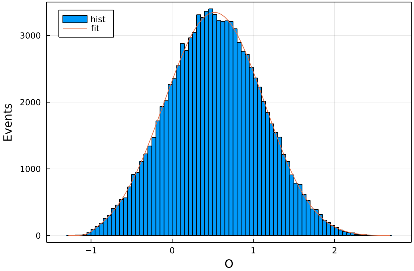
# SU3 example

- $S = Re[Tr(U) - 1]^2$
- $O = Re[Tr(U)]$
- $D = 1$
- Fitted with spline of order 20, but too smooth, due to pole at $O = -1$
- Table Shows results from extrapolating with 3rd order polynomial in small area around O

| N | Observable | Re | Im |
|---|---|---|---|
| $10^5$ | O | $0.5313 \pm 0.0094$ | 0 |
| $10^6$ | O | $0.5194 \pm 0.0037$ | 0 |
| $10^5$ | dV | $0.5244 \pm 0.0002$ | 0 |
| $10^6$ | dV | $0.5242 \pm 0.00009$ | 0 |

Table: Results for different amount of samples.



# Wilson Lines

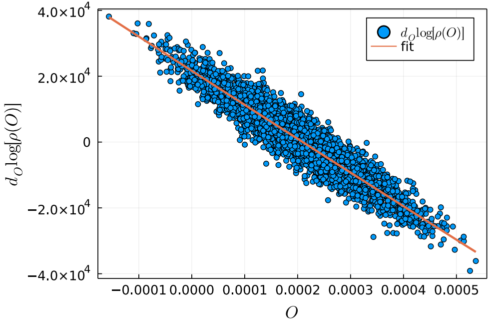
- The wilson line correlator is defined as

$$C(\tau, r) \quad = \quad \sum_{\tau', x} Tr[(\Pi_{j=0}^{\tau/a-1} U_4(\tau' + aj, x))(\Pi_{j=0}^{\tau/a-1} U_4(\tau' + aj, x + r))^\dagger] \tag{15}$$

- multiplications starts to the left and then move to the right.
- We have

$$C(\tau, r) = C(\tau, -r)^\dagger \tag{16}$$

- Configurations needs to be gauge fixed



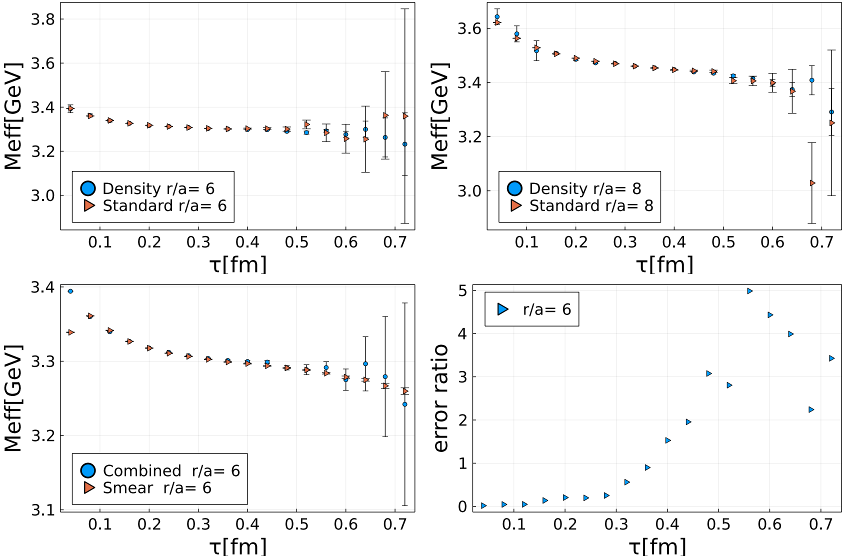
# Setup

- $\partial_{x_i} S$ is taken from the Hybrid-Monte-Carlo simulation code from which the configurations were generated. In this case it is SIMULATeQCD.
- HISQ configurations of size $64^3 20$ for $\beta = 7.825$, $a = 0.04fm$, $T = 244MeV$ and $m_s/m_l = 20$, $N_{conf} = 4400$.
- Distribution close to gaussian since each observable average over entire volume
- Fitted with second order polynomial to $d_O \log(\rho)$
- Third order checked, but not significant
- From the found correlation functions we plot the effective mass

$$M_{eff}(\tau) = \frac{1}{a}\log(C(\tau)/C(\tau+1)) \tag{17}$$

- Might be a derivative on gauge fixing which is not taken into account

# Wilson Lines Results



# Conclusion

- Derived formula for change to the density of an observable

$$\frac{d\log(\rho(O))}{dO} = \langle \frac{O_{i,i}}{O_j^2} - \frac{2O_iO_{i,j}O_j}{(O_k^2)^2} - \frac{S_iO_i}{O_j^2} \rangle \quad (18)$$

- Showed results from using the formula in a range of different examples
- Improvements found in many cases, though not always and can be expensive to calculate for some observables