

1 Hamiltonian Monte Carlo for fuzzy spaces

1.1 Statement of the problem

The fuzzy space action considered here is:

$$S[D] = g_2 \operatorname{Tr} D^2 + \operatorname{Tr} D^4 \quad (1)$$

where $g_2 \in \mathbb{R}$ and D is of the form:

$$D = \sum_i \omega_i \otimes (M_i \otimes I + \epsilon_i I \otimes M_i^T) \quad (2)$$

for Hermitian ω_i and M_i , and $\epsilon_i = \pm 1$.

The dynamical variables in the Monte Carlo are the $n \times n$ matrices M_i .

Hamiltonian Monte Carlo requires to take derivatives such as:

$$\frac{\partial S[M_i]}{\partial M_k} \quad (3)$$

which amounts to finding formulas for terms like:

$$\frac{\partial \operatorname{Tr} D^p}{\partial M_k}. \quad (4)$$

In the following, formulas for $p = 2$ and $p = 4$ are developed.

1.2 Matrix calculus

Let $A \in M_n(\mathbb{C})$ and $f(A)$ be a complex valued function of A . The derivative of f with respect to A is defined in components as the $n \times n$ matrix:

$$\left(\frac{\partial f}{\partial A} \right)_{lm} \equiv \frac{\partial f}{\partial A_{lm}}. \quad (5)$$

The two special cases of interest here are:

$$\frac{\partial \operatorname{Tr} A}{\partial A} = I \quad (6)$$

$$\frac{\partial \operatorname{Tr} AB}{\partial A} = B^T. \quad (7)$$

1.3 The case $p = 2$

When $p = 2$ the M_i matrices are decoupled:

$$\text{Tr } D^2 = \sum_i \text{Tr } \omega_i^2 (2n \text{Tr } M_i^2 + 2\epsilon_i (\text{Tr } M_i)^2). \quad (8)$$

Taking a derivative with respect to M_k yields:

$$\begin{aligned} \frac{\partial}{\partial M_k} \left(\sum_i \text{Tr } \omega_i^2 (2n \text{Tr } M_i^2 + 2\epsilon_i (\text{Tr } M_i)^2) \right) = \\ \sum_i \delta_{ik} \text{Tr } \omega_i^2 (4n M_i^T + 4\epsilon_i (\text{Tr } M_i) I) = \\ 4C (n M_k^T + \epsilon_k (\text{Tr } M_k) I) \end{aligned} \quad (9)$$

where $C \equiv \text{Tr } \omega_i^2$ is the dimension of the Clifford module.

1.4 The case $p = 4$

First expand $\text{Tr } D^4$:

$$\begin{aligned} \text{Tr } D^4 = \sum_{i_1, i_2, i_3, i_4} \text{Tr}(\omega_{i_1} \omega_{i_2} \omega_{i_3} \omega_{i_4}) \cdot \\ \left(n[1 + \epsilon *] \text{Tr}(M_{i_1} M_{i_2} M_{i_3} M_{i_4}) + \right. \\ \epsilon_{i_1} \text{Tr } M_{i_1} [1 + \epsilon *] \text{Tr}(M_{i_2} M_{i_3} M_{i_4}) + \\ \epsilon_{i_2} \text{Tr } M_{i_2} [1 + \epsilon *] \text{Tr}(M_{i_1} M_{i_3} M_{i_4}) + \\ \epsilon_{i_3} \text{Tr } M_{i_3} [1 + \epsilon *] \text{Tr}(M_{i_1} M_{i_2} M_{i_4}) + \\ \epsilon_{i_4} \text{Tr } M_{i_4} [1 + \epsilon *] \text{Tr}(M_{i_1} M_{i_2} M_{i_3}) + \\ \epsilon_{i_1} \epsilon_{i_2} [1 + \epsilon] \text{Tr}(M_{i_1} M_{i_2}) \text{Tr}(M_{i_3} M_{i_4}) + \\ \epsilon_{i_1} \epsilon_{i_3} [1 + \epsilon] \text{Tr}(M_{i_1} M_{i_3}) \text{Tr}(M_{i_2} M_{i_4}) + \\ \left. \epsilon_{i_1} \epsilon_{i_4} [1 + \epsilon] \text{Tr}(M_{i_1} M_{i_4}) \text{Tr}(M_{i_2} M_{i_3}) \right) \end{aligned} \quad (10)$$

where $*$ denotes complex conjugation of everything that appears on the right, ϵ is defined as the product $\epsilon \equiv \epsilon_{i_1} \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4}$, and the relation $M^T = M^*$ has been used. The reality of the expression comes from the fact that a simultaneous index exchange $i_1 \leftrightarrow i_4$ and $i_2 \leftrightarrow i_3$ is equivalent to taking the complex

conjugate.

Taking a matrix derivative with respect to M_k results in non-vanishing contributions when $k = i_1, k = i_2, k = i_3$ or $k = i_4$:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 = \sum_{i_1, i_2, i_3, i_4} \text{Tr}(\omega_{i_1} \omega_{i_2} \omega_{i_3} \omega_{i_4}) \cdot \\ \left(\delta_{ki_1} A(i_1, i_2, i_3, i_4)^T + \delta_{ki_2} A(i_2, i_3, i_4, i_1)^T + \right. \\ \left. \delta_{ki_3} A(i_3, i_4, i_1, i_2)^T + \delta_{ki_4} A(i_4, i_1, i_2, i_3)^T \right) \end{aligned} \quad (11)$$

where $A(a, b, c, d)$ is the following $n \times n$ matrix:

$$\begin{aligned} A(a, b, c, d) \equiv n[1 + \epsilon \dagger] M_b M_c M_d + \\ \epsilon_a I[1 + \epsilon *] \text{Tr } M_b M_c M_d + \\ \epsilon_b \text{Tr } M_b [1 + \epsilon \dagger] M_c M_d + \\ \epsilon_c \text{Tr } M_c [1 + \epsilon \dagger] M_b M_d + \\ \epsilon_d \text{Tr } M_d [1 + \epsilon \dagger] M_b M_c + \\ \epsilon_a \epsilon_b M_b [1 + \epsilon] \text{Tr } M_c M_d + \\ \epsilon_a \epsilon_c M_c [1 + \epsilon] \text{Tr } M_b M_d + \\ \epsilon_a \epsilon_d M_d [1 + \epsilon] \text{Tr } M_b M_c \end{aligned} \quad (12)$$

Where \dagger denotes Hermitian conjugation of everything that appears on the right.

Now it is useful to write Eq.(11) symbolically as:

$$\frac{\partial}{\partial M_k} \text{Tr } D^4 = \sum_{i_1, i_2, i_3, i_4} \mathcal{B}(i_1, i_2, i_3, i_4) \quad (13)$$

and notice that a simultaneous exchange of indices $i_1 \leftrightarrow i_4$ and $i_2 \leftrightarrow i_3$ is equivalent to taking the Hermitian conjugate:

$$\mathcal{B}(i_1, i_2, i_3, i_4)^\dagger = \mathcal{B}(i_4, i_3, i_2, i_1). \quad (14)$$

One can then introduce an equivalence relation $(i_1, i_2, i_3, i_4) \sim (i_4, i_3, i_2, i_1)$ and restrict the sum on the equivalence classes:

$$\frac{\partial}{\partial M_k} \text{Tr } D^4 = \sum_{[i_1, i_2, i_3, i_4]} \frac{|[i_1, i_2, i_3, i_4]|}{2} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) \quad (15)$$

where \dagger denotes Hermitian conjugation of everything that appears on the right, and the factor $||[i_1, i_2, i_3, i_4]||/2$ involving the cardinality of the class prevents from overcounting terms of the type $\mathcal{B}(i_1, i_2, i_2, i_1)$.

The truncated sum can be written explicitly in the following way:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 = & \sum_{\substack{i_4 < i_1 \\ i_3 < i_2}} [1 + \dagger] (\mathcal{B}(i_1, i_2, i_3, i_4) + \mathcal{B}(i_1, i_3, i_2, i_4)) + \\ & \sum_{\substack{i_4 = i_1 \\ i_3 < i_2}} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) + \sum_{\substack{i_4 < i_1 \\ i_3 = i_2}} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) + \\ & \sum_{\substack{i_4 = i_1 \\ i_3 = i_2}} \mathcal{B}(i_1, i_2, i_3, i_4) \end{aligned} \quad (16)$$

Moreover notice that the second line vanishes due to the properties of the ω matrices:

$$\text{Tr}(\omega_{\sigma(i_1)} \omega_{\sigma(i_2)} \omega_{\sigma(j)} \omega_{\sigma(k)}) \sim \text{Tr}(\omega_j \omega_k) = 0 \quad \text{if } i_1 = i_2 \text{ and } j \neq k \quad (17)$$

for any permutation σ acting on $\{i_1, i_2, j, k\}$.

Therefore Eq.(16) simplifies to:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 = & \sum_{\substack{i_4 < i_1 \\ i_3 < i_2}} [1 + \dagger] (\mathcal{B}(i_1, i_2, i_3, i_4) + \mathcal{B}(i_1, i_3, i_2, i_4)) + \sum_{i_1, i_2} \mathcal{B}(i_1, i_2, i_2, i_1) \end{aligned} \quad (18)$$

which is a Hermitian matrix.

1.5 A general formula for every p

The first problem is to write $\text{Tr } D^p$ in a useful form, along the lines of Eq.(10).

$\text{Tr } D^p$ expands to:

$$\begin{aligned} \text{Tr } D^p = & \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \cdot \\ & \text{Tr} \left((M_{i_1} \otimes I + \epsilon_{i_1} I \otimes M_{i_1}^T) \dots (M_{i_p} \otimes I + \epsilon_{i_p} I \otimes M_{i_p}^T) \right) \end{aligned} \quad (19)$$

Ignoring (for now) the trace over the ω matrices, a typical term in the sum is:

$$\text{Tr} (\epsilon_B A \otimes B^* + \epsilon_A B \otimes A^*) \quad (20)$$

where A and B are related to the product $M_{i_1} \dots M_{i_p}$ in the following way:

1. pick $r \geq 0$ numbers $k_1 < \dots < k_r$ from $\{1, \dots, p\}$ and call the remaining $p - r$ numbers $j_1 < \dots < j_{p-r}$;
2. define $A = M_{i_{k_1}} \dots M_{i_{k_r}}$ and $B = M_{i_{j_1}} \dots M_{i_{j_{p-r}}}$ (if $r = 0$, $A = I$);
3. define $\epsilon_A = \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}}$ and $\epsilon_B = \epsilon_{i_{j_1}} \dots \epsilon_{i_{j_{p-r}}} = \epsilon_A \epsilon_{i_1} \dots \epsilon_{i_p}$.

In particular, a choice of A completely characterizes B .

By varying r from 0 to $\lfloor \frac{p}{2} \rfloor$ and summing over all possible choices of $k_1 \dots k_r$, every term in $\text{Tr} D^p$ is generated.

One can verify that every term in Eq.(10) ($p = 4$) is of that type. For example:

$$\begin{aligned} \text{Tr} M_{i_1} [\epsilon_{i_1} + \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} *] \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) = \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr} M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr} M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) = \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr} M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr} (M_{i_1})^* \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) = \\ \text{Tr} (\epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} M_{i_1} \otimes (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} M_{i_2} M_{i_3} M_{i_4} \otimes M_{i_1}^*) \end{aligned} \quad (21)$$

which is of the form of Eq.(20) upon identifying M_{i_1} with A and $M_{i_2} M_{i_3} M_{i_4}$ with B (in the second equality the reality of $\text{Tr} M_{i_1}$ has been used).

A way of expressing $\text{Tr} B$ given A is using a modified derivative operator D_i defined as:

$$D_i \equiv \text{Tr} \circ \frac{\partial}{\partial M_i} \quad (22)$$

which allows to write:

$$A = M_{i_{k_1}} \dots M_{i_{k_r}} \implies \text{Tr} B = D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr} (M_{i_1} \dots M_{i_p}). \quad (23)$$

Therefore Eq.(20) becomes:

$$\begin{aligned} \epsilon_A [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr} A)^* \text{Tr} B = \\ \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr} M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr} (M_{i_1} \dots M_{i_p})). \end{aligned} \quad (24)$$

There are some special cases that make the expression simpler, namely:

1. $r = 0$ gives a factor $\text{Tr } I = n$;
2. $r = 1, 2$ make $\text{Tr } A$ real;
3. $p - r = 1, 2$ (which can only occur for $p = 2, 4$) make $\text{Tr } B$ real.

Putting everything together, $\text{Tr } D^p$ can be written as:

$$\text{Tr } D^p = \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \left[\sum_{r=0}^{\left[\frac{p}{2}\right]} \sum_{k_1 < \dots < k_r=1}^p \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \right. \\ \left. (\text{Tr } M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p})) \right]. \quad (25)$$

where:

$$r = 0 \quad \longrightarrow \quad n[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \text{Tr}(M_{i_1} \dots M_{i_p}) \quad (26)$$

$$r = 1 \quad \longrightarrow \quad \sum_{k_1=1}^p \epsilon_{i_{k_1}} \text{Tr}(M_{i_{k_1}})[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}) \quad (27)$$

$$r = 2 \quad \longrightarrow \quad \sum_{k_1 < k_2=1}^p \epsilon_{i_{k_1}} \epsilon_{i_{k_2}} \text{Tr}(M_{i_{k_1}} M_{i_{k_2}})[1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] D_{i_{k_2}} D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}). \quad (28)$$