

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. Since D is Hermitian, the expression must be real. It is not immediate to see that this is the case because of the $\epsilon = \pm 1$ factor inside

the square brackets. Reality nonetheless holds, and becomes manifest by observing that a simultaneous index exchange $i_1 \leftrightarrow i_4$ and $i_2 \leftrightarrow i_3$ is equivalent to taking the complex conjugate (in fact, this is not the only index exchange that amounts to complex conjugation).

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 $k = i_4$:

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

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

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

and \dagger denotes Hermitian conjugation of everything that appears on the right. Upon relabeling the indices and cycling the ω matrices in the trace, the equation becomes:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 &= 4 \sum_{i_1, i_2, i_3, i_4} \delta_{ki_1} \text{Tr}(\omega_{i_1} \omega_{i_2} \omega_{i_3} \omega_{i_4}) A(i_1, i_2, i_3, i_4)^T \\ &= 4 \sum_{i_1, i_2, i_3} \text{Tr}(\omega_k \omega_{i_1} \omega_{i_2} \omega_{i_3}) A(k, i_1, i_2, i_3)^T \equiv 4 \sum_{i_1, i_2, i_3} \mathcal{B}_k(i_1, i_2, i_3) \end{aligned} \quad (13)$$

with $\mathcal{B}_k(a, b, c)$ denoting the generic term in the sum.

To see that Eq.(13) defines a Hermitian matrix, notice that an exchange of

indices $i_1 \leftrightarrow i_3$ is equivalent to taking the Hermitian conjugate:

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

therefore Eq.(13) reduces to:

$$\sum_{\substack{i_1 > i_3 \\ i_2}} [1 + \dagger] \mathcal{B}_k(i_1, i_2, i_3) + \sum_{i_1, i_2} \mathcal{B}_k(i_1, i_2, i_1). \quad (15)$$

In fact, by looking at the form of \mathcal{B} , it is clear that terms in the sum are qualitatively different based on the number of indices that coincide. Therefore it would be computationally convenient to write Eq.(15) in a way that emphasises this difference.

The only terms that contribute when all indices are different are the following:

$$\sum_{i_1 > i_2 > i_3} [1 + \dagger] \left(\mathcal{B}_k(i_1, i_2, i_3) + \mathcal{B}_k(i_1, i_3, i_2) + \mathcal{B}_k(i_2, i_1, i_3) \right). \quad (16)$$

The three inequivalent permutations of indices that appear in this formula are based on a group-theoretical argument that will generalize easily to powers of D higher than 4. First consider the symmetric group of order three S_3 acting on the set of indices $\{i_1, i_2, i_3\}$, and the subgroup of permutations that induce a simple change in \mathcal{B} , which in this case is $H = \{(), (13)\} \cong S_2$ (the first element being the identical permutation, and the second the exchange $i_1 \leftrightarrow i_3$ which induces $\mathcal{B} \rightarrow \mathcal{B}^\dagger$). The idea is then to restrict the sum to $i_1 > i_2 > i_3$ and quotient out the action of H by introducing a suitable pre-factor that accounts for it (in this case $[1 + \dagger]$). Practically, the inequivalent permutations of indices that appear in Eq.(16) are found by computing the (left or right) cosets of $H \subset S_3$ and acting on $\{i_1, i_2, i_3\}$ with a representative from each coset. In this case the representatives were chosen to be $()$, (23) , (12) .

What is left are terms in which at least two indices are equal. These are:

$$\begin{aligned} \sum_{i_1 > i_2} [1 + \dagger] \left(\mathcal{B}_k(i_1, i_1, i_2) + \mathcal{B}_k(i_1, i_2, i_2) \right) + \\ \sum_{i_1 \neq i_2} \mathcal{B}_k(i_1, i_2, i_1) + \sum_i \mathcal{B}_k(i, i, i). \end{aligned} \quad (17)$$

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:

$$\begin{aligned} \text{Tr } D^p &= \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \cdot \\ &\text{Tr} \left((M_{i_1} \otimes I + \epsilon_{i_1} I \otimes M_{i_1}^T) \dots (M_{i_p} \otimes I + \epsilon_{i_p} I \otimes M_{i_p}^T) \right) \end{aligned} \quad (18)$$

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

$$\text{Tr} (\epsilon_B A \otimes B^* + \epsilon_A B \otimes A^*) \quad (19)$$

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:

$$\begin{aligned} \text{Tr } M_{i_1} [\epsilon_{i_1} + \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4}^*] \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr} (M_{i_1})^* \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \text{Tr} (\epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} M_{i_1} \otimes (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} M_{i_2} M_{i_3} M_{i_4} \otimes M_{i_1}^*) & \end{aligned} \quad (20)$$

which is of the form of Eq.(19) 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:

$$D_i \equiv \text{Tr} \circ \frac{\partial}{\partial M_i} \quad (21)$$

which allows to write:

$$A = M_{i_{k_1}} \dots M_{i_{k_r}} \implies \text{Tr } B = D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}). \quad (22)$$

Therefore Eq.(19) becomes:

$$\begin{aligned} \epsilon_A [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr } A)^* \text{Tr } B = \\ \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr } M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p})). \end{aligned} \quad (23)$$

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:

$$\begin{aligned} \text{Tr } D^p = \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \left[\sum_{r=0}^{\left[\frac{p}{2}\right]} \sum_{k_1 < \dots < k_r=1}^p \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \right. \\ \left. (\text{Tr } M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p})) \right]. \end{aligned} \quad (24)$$

where:

$$r = 0 \longrightarrow n [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \text{Tr}(M_{i_1} \dots M_{i_p}) \quad (25)$$

$$r = 1 \longrightarrow \sum_{k_1=1}^p \epsilon_{i_{k_1}} \text{Tr}(M_{i_{k_1}}) [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}) \quad (26)$$

$$r = 2 \longrightarrow \sum_{k_1 < k_2=1}^p \epsilon_{i_{k_1}} \epsilon_{i_{k_2}} \text{Tr}(M_{i_{k_1}} M_{i_{k_2}}) [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] D_{i_{k_2}} D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}). \quad (27)$$