

# 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  $\omega_i$  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,  $\epsilon$  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 presence of  $\epsilon = \pm 1$  inside the square brackets spoils the otherwise manifest reality of the expression, which instead 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:

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

and  $\dagger$  denotes Hermitian conjugation of everything that appears on the right. Again Eq.(11) does not look manifestly Hermitian because of the  $\epsilon$  factor in the square brackets. To see that this is indeed the case, 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  $i_2 \leftrightarrow i_3$  (call this permutation  $\rho$ ) is equivalent to taking the Hermitian conjugate:

$$\mathcal{B}(i_1, i_2, i_3, i_4)^\dagger = \mathcal{B}(i_{\rho(1)}, i_{\rho(2)}, i_{\rho(3)}, i_{\rho(4)}) = \mathcal{B}(i_4, i_3, i_2, i_1). \quad (14)$$

This property can also be exploited to gain some computational efficiency. One can introduce an equivalence relation

$$(i_1, i_2, i_3, i_4) \sim (i_{\rho^m(1)}, i_{\rho^m(2)}, i_{\rho^m(3)}, i_{\rho^m(4)}), \quad m \in \mathbb{N} \quad (15)$$

and restrict the sum on the equivalence classes:

$$\frac{\partial}{\partial M_k} \text{Tr } D^4 = \sum_{[i_1, i_2, i_3, i_4]} \frac{|[i_1, i_2, i_3, i_4]|}{2} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) \quad (16)$$

where  $|[i_1, i_2, i_3, i_4]|$  is the cardinality of the class. Practically,  $\rho^{2m}$  is the identity permutation, and the equivalence classes have one or two elements. The factor involving the cardinality of the class prevents from overcounting terms of the type  $(a, b, b, a)$  (which are the only elements with class of cardinality one).

The sum of Eq.(16) can be written explicitly in the following way:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 = & \sum_{\substack{i_4 < i_1 \\ i_3 < i_2}} [1 + \dagger] (\mathcal{B}(i_1, i_2, i_3, i_4) + \mathcal{B}(i_1, i_3, i_2, i_4)) + \\ & \sum_{\substack{i_4 = i_1 \\ i_3 < i_2}} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) + \sum_{\substack{i_4 < i_1 \\ i_3 = i_2}} [1 + \dagger] \mathcal{B}(i_1, i_2, i_3, i_4) + \\ & \sum_{\substack{i_4 = i_1 \\ i_3 = i_2}} \mathcal{B}(i_1, i_2, i_3, i_4) \end{aligned} \quad (17)$$

and simplified noticing that the second line vanishes due to the properties of the  $\omega$  matrices:

$$\text{Tr}(\omega_{\sigma(i_1)} \omega_{\sigma(i_2)} \omega_{\sigma(j)} \omega_{\sigma(k)}) \propto \text{Tr}(\omega_j \omega_k) = 0 \quad \text{if } i_1 = i_2 \text{ and } j \neq k \quad (18)$$

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

Therefore Eq.(17) simplifies to:

$$\begin{aligned} \frac{\partial}{\partial M_k} \text{Tr } D^4 = & \sum_{\substack{i_4 < i_1 \\ i_3 < i_2}} [1 + \dagger] (\mathcal{B}(i_1, i_2, i_3, i_4) + \mathcal{B}(i_1, i_3, i_2, i_4)) + \sum_{i_1, i_2} \mathcal{B}(i_1, i_2, i_2, i_1). \end{aligned} \quad (19)$$

For the same reason, terms in the first sum for which  $(i_1 = i_2 \text{ and } i_3 \neq i_4)$  or  $(i_1 = i_3 \text{ and } i_2 \neq i_4)$  need not be computed as they vanish.

## 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:

$$\begin{aligned} \text{Tr } D^p &= \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \cdot \\ &\text{Tr} \left( (M_{i_1} \otimes I + \epsilon_{i_1} I \otimes M_{i_1}^T) \dots (M_{i_p} \otimes I + \epsilon_{i_p} I \otimes M_{i_p}^T) \right) \end{aligned} \quad (20)$$

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

$$\text{Tr} (\epsilon_B A \otimes B^* + \epsilon_A B \otimes A^*) \quad (21)$$

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:

$$\begin{aligned} \text{Tr } M_{i_1} [\epsilon_{i_1} + \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4}^*] \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} \text{Tr } M_{i_1} \text{Tr} (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} \text{Tr} (M_{i_1})^* \text{Tr} (M_{i_2} M_{i_3} M_{i_4}) &= \\ \text{Tr} (\epsilon_{i_2} \epsilon_{i_3} \epsilon_{i_4} M_{i_1} \otimes (M_{i_2} M_{i_3} M_{i_4})^* + \epsilon_{i_1} M_{i_2} M_{i_3} M_{i_4} \otimes M_{i_1}^*) & \end{aligned} \quad (22)$$

which is of the form of Eq.(21) 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:

$$D_i \equiv \text{Tr} \circ \frac{\partial}{\partial M_i} \quad (23)$$

which allows to write:

$$A = M_{i_{k_1}} \dots M_{i_{k_r}} \implies \text{Tr } B = D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}). \quad (24)$$

Therefore Eq.(21) becomes:

$$\begin{aligned} \epsilon_A [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr } A)^* \text{Tr } B = \\ \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] (\text{Tr } M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p})). \end{aligned} \quad (25)$$

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:

$$\begin{aligned} \text{Tr } D^p = \sum_{i_1 \dots i_p} \text{Tr } \omega_{i_1} \dots \omega_{i_p} \left[ \sum_{r=0}^{\left\lfloor \frac{p}{2} \right\rfloor} \sum_{k_1 < \dots < k_r=1}^p \epsilon_{i_{k_1}} \dots \epsilon_{i_{k_r}} [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \right. \\ \left. (\text{Tr } M_{i_{k_1}} \dots M_{i_{k_r}})^* (D_{i_{k_r}} \dots D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p})) \right]. \end{aligned} \quad (26)$$

where:

$$r = 0 \longrightarrow n [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] \text{Tr}(M_{i_1} \dots M_{i_p}) \quad (27)$$

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

$$r = 2 \longrightarrow \sum_{k_1 < k_2=1}^p \epsilon_{i_{k_1}} \epsilon_{i_{k_2}} \text{Tr}(M_{i_{k_1}} M_{i_{k_2}}) [1 + \epsilon_{i_1} \dots \epsilon_{i_p} *] D_{i_{k_2}} D_{i_{k_1}} \text{Tr}(M_{i_1} \dots M_{i_p}). \quad (29)$$