Notes on smearing

Albert Deuzeman

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Abstract

This working document gives the derivation of the different smearing schemes in use in the tmLQCD code.

1 Introduction

As a basis of our treatment of smearing, we will use the framework of the BMW collaboration. In their paper with analysis details of the HEX-smeared simulations, they work out the equations that describe the transportation of variations in an underlying gaugefield through an (analytic) smearing procedure. We will not repeat their generic derivation here, but just quote their master equation

$$\frac{\delta S}{\delta U} \equiv \frac{\delta S}{\delta V} \star \frac{\delta V}{\delta U} = P_{\mathrm{TA}} \left[U \left[V^{\dagger} \frac{\delta S}{\delta V} \right]_{ab} \frac{\partial V_{ba}}{\partial U} \right]. \tag{1}$$

We can unroll several levels of smearing by applying this formula iteratively, but we need to specify the implementation of this equation for each specific smearing scheme. That specification is the purpose of this document.

In the following, we'll need the 'plain derivative' of matrices. One can go about this in several ways, but for the purpose of ease of implementation we'll skip the compact index-free notation and instead go for explicit indices on our matrices. The identities we'll need are

$$\frac{\partial U(\mu, x)_{ab}}{\partial U(\nu, y)_{cd}} = \delta(x, y)\delta(\mu, \nu) I_{ca} I_{bd} \tag{2}$$

and[1]

$$\frac{\partial U^{\dagger}(\mu, x)_{ab}}{\partial U(\nu, y)_{cd}} = -\delta(x, y)\delta(\mu, \nu) U(x, \mu)^{\dagger}_{ca} U(x, \mu)^{\dagger}_{bd}. \tag{3}$$

2 Stout smearing

Our first port of call is the classical stout smearing according to Peardon and Morningstar. They explicitly give results for the smearing of forces in an HMC

[1] Use the regular chain rule to find

$$\frac{\partial (U^{\dagger} U)}{\partial A} = \frac{\partial U^{\dagger}}{\partial A} U + U^{\dagger} \frac{\partial U}{\partial A} = \frac{\partial I}{\partial A} = 0.$$

Solve for the derivative of the hermitian transpose.

setup, but we want to reproduce those within BMW's framework. Since most of this derivation is identical to that of HEX smearing, we can follow BMW's lead and write

$$\frac{\delta S}{\delta U} = P_{\mathrm{TA}} \left(U \Sigma_{ab} \frac{\partial V_{ab}}{\partial U} \right), \tag{4}$$

introducing the shorthand notation

$$\left[V^\dagger \frac{\delta S}{\delta V} \right]_{ab} \equiv \Sigma_{ab}. \tag{5}$$

In the case of stouting, we have the relationship

$$V = \exp(P_{\mathrm{TA}} \left[C U^\dagger \right]) U \equiv \exp\left[A\right] U, \tag{6}$$

so the common chain rule gives

$$\frac{\delta S}{\delta U} = P_{\mathrm{TA}} \left(U \Sigma_{ab} \frac{\partial \exp\left[A\right]_{bc}}{\partial U} U_{ca} \right) + P_{\mathrm{TA}} \left(U \Sigma_{ab} \exp\left[A\right]_{ba} \right). \tag{7}$$

The second term is straightforward to calculate. For the first, we can use the derivation by Peardon and Morningstar and obtain

$$P_{\mathrm{TA}} \left(U \Sigma_{ab} \frac{\partial \exp\left[A\right]_{bc}}{\partial U} U_{ca} \right) =$$
$$P_{\mathrm{TA}} \left(U \frac{\partial A_{ab}}{\partial U} \left[\mathrm{Tr}\left(U \Sigma B_1 \right) A + \mathrm{Tr}\left(U \Sigma B_2 \right) A^2 + f_1 U \Sigma + f_2 \left(U \Sigma A + A U \Sigma \right) \right]_{ba} \right) \tag{8}$$

We now need the derivative

$$\frac{\partial A_{ab}}{\partial U} = \frac{\partial P_{\mathrm{TA}}(C U^\dagger)}{\partial U}, \tag{9}$$

which we can fortunately simplify by moving the projector P_{TA} to the term it multiplies. We can then write

$$U \frac{\partial (C U^\dagger)_{ab}}{\partial U} = U \frac{\partial C_{ab}}{\partial U} \left(U^\dagger P_{\mathrm{TA}} \left[\ldots \right] \right)_{ba} - P_{\mathrm{TA}} \left[\ldots \right] C U^\dagger \tag{10}$$

At this point, BMW introduces the notation

$$Z_{\mathrm{ba}} =$$
$$U^\dagger_{bc} P_{\mathrm{TA}} \left[\mathrm{Tr}\left(U \Sigma B_1 \right) A + \mathrm{Tr}\left(U \Sigma B_2 \right) A^2 + f_1 U \Sigma + f_2 \left(U \Sigma A + A U \Sigma \right) \right]_{ca}, \tag{11}$$

giving us the more manageable expression[2]

$$\frac{\delta S}{\delta U} = P_{\mathrm{TA}} \left(U \left(\Sigma V - Z C \right) U^\dagger + U \frac{\partial C_{ab}}{\partial U} Z_{ba} \right). \tag{12}$$

So far so good! All that was used was the exponential nature of the smearing. But at this point, HEX smearing and stout smearing start to deviate. HEX

[2]Using the identity $\exp A = V U^\dagger$.

smearing needs three iterations around the same background with selected staples. Stout smearing has a fully symmetric set of staples and produces V in a single step. That means all we should need is the staple derivative term. Since this is a tricky derivation, let's add all the indices we've been suppressing so far

$$U(\sigma, y)_{cd} \frac{\partial C(\sigma, y)_{ab}}{\partial U(\mu, x)_{de}} Z(\sigma, y)_{ba}.$$

We should now plug in the details of the staple construction $C(\sigma, y)_{ab}$

$$\begin{aligned} C(\sigma, y)_{ab} Z(\sigma, y)_{ba} = \rho \sum_{\tau \neq \sigma} \Big(& U(\tau,\, y)_{ap} U(\sigma,\, y + \hat{\tau})_{pq} U^\dagger(\tau,\, y + \hat{\sigma})_{qb} Z(\sigma, y)_{ba} \\ & + U^\dagger(\tau,\, y - \hat{\tau})_{ap} U(\sigma,\, y - \hat{\tau})_{pq} U(\tau,\, y - \hat{\tau} + \hat{\sigma})_{qb} Z(\sigma, y)_{ba} \Big). \end{aligned} \tag{13}$$

Operating on this with the derivative gives

$$\begin{aligned} \frac{\partial C(\sigma, y)_{ab}}{\partial U(\mu, x)_{de}} Z(\sigma, y)_{ba} = & \\ \rho \sum_{\nu \neq \mu} \Big(& U(\nu,\, x + \hat{\mu})_{dq} U^\dagger(\mu,\, x + \hat{\nu})_{qb} Z(\nu, x)_{be} \\ & + U^\dagger(\nu,\, x - \hat{\nu} + \hat{\mu})_{db} Z(\mu, x - \hat{\nu})_{ba} U(\nu,\, x - \hat{\nu})_{ae} \\ & - U^\dagger(\mu,\, x)_{db} Z(\nu, x - \hat{\nu})_{ba} U(\mu,\, x - \hat{\nu})_{ap} U(\nu,\, x - \hat{\nu} + \hat{\mu})_{pq} U^\dagger(\mu,\, x)_{qe} \\ & - U^\dagger(\mu,\, x)_{dp} U(\nu,\, x)_{pq} U(\mu,\, x + \hat{\nu})_{qb} Z(\nu, x + \hat{\mu})_{ba} U^\dagger(\mu,\, x)_{ae} \\ & + U(\nu,\, x + \hat{\mu})_{db} Z(\mu, x + \hat{\nu})_{ba} U^\dagger(\nu,\, x)_{ae} \\ & + Z(\nu, x + \hat{\mu} - \hat{\nu})_{da} U^\dagger(\mu,\, x - \hat{\nu})_{ap} U(\nu,\, x - \hat{\nu})_{pe} \Big). \end{aligned} \tag{14}$$

Comparing this to the expression of Peardon and Morningstar, there is clear agreement in all the positive terms. Differences appear when it comes to the derivatives of the hermitian conjugate terms. There, Peardon and Morningstar seem to use

$$U_1 \frac{\partial U_2^\dagger}{\partial U} U_3 U_\Lambda \Lambda = (U_1 U_3 U_\Lambda \Lambda)^\dagger = -\Lambda U_\Lambda^\dagger U_1^\dagger U_3^\dagger, \tag{15}$$

where the notation is somewhat approximate and we use the fact that Λ is antihermitian. This discrepancy is just noted here for potential future reference. For implementation purposes, we can clear up equation 14 and add the missing multiplication by $U_{cd}(\mu, x)$ to obtain

$$
\begin{aligned}
U(\mu,x)_{cd}\frac{\partial C(\sigma,y)_{ab}}{\partial U(\mu,x)_{de}}Z(\sigma,y)_{ba} = \\
\rho\sum_{\nu\neq\mu}\Big(& U(\mu,x)U(\nu,\, x+\hat{\mu})U^{\dagger}(\mu,\, x+\hat{\nu})Z(\nu,x) \\
& + U(\mu,x)U^{\dagger}(\nu,\, x-\hat{\nu}+\hat{\mu})Z(\mu,x-\hat{\nu})U(\nu,\, x-\hat{\nu}) \\
& - Z(\nu,x-\hat{\nu})U(\mu,\, x-\hat{\nu})U(\nu,\, x-\hat{\nu}+\hat{\mu})U^{\dagger}(\mu,\, x) \\
& - U(\nu,\, x)U(\mu,\, x+\hat{\nu})Z(\nu,x+\hat{\mu})U^{\dagger}(\mu,\, x) \\
& + U(\mu,x)U(\nu,\, x+\hat{\mu})Z(\mu,x+\hat{\nu})U^{\dagger}(\nu,\, x) \\
& + U(\mu,x)Z(\nu,x+\hat{\mu}-\hat{\nu})U^{\dagger}(\mu,\, x-\hat{\nu})U(\nu,\, x-\hat{\nu})\Big).
\end{aligned}
\tag{16}
$$