

Supplementary Material for the Paper: An Interface between Grassmann manifolds and vector spaces

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1. Gradient computation of the Grassmann Log Map

In this document, we present a derivation of the gradient of the log map for the Grassmann manifold $\mathcal{G}(d, m)$. For that, we utilise various conventional techniques to operate differential forms [1].

Given the data and the loss gradient $\nabla_H L = \dot{H}$, we compute the gradients with respect to the tangency point and data.

The Grassmann log consists of the three equations below:

$$B = (K^\top X)^{-1}(K^\top - K^\top X X^\top), \quad (1)$$

$$W\Theta Z^\top = B^\top, \quad (2)$$

$$\text{Log}_K X = H = W^* \arctan(\Theta^*) Z^{*\top}, \quad (3)$$

where W^* , Θ^* , Z^* represent the matrices with the first m columns of W , Θ and Z respectively. It should be noted that equation 2 is the transposed SVD of B . The differential of the expression 3 may be written as:

$$H = W^* \arctan(\Theta^*) Z^{*\top} = W^* S Z^{*\top}, \quad (4)$$

$$dH = dW^* S Z^{*\top} + W^* dS Z^{*\top} + W^* S dZ^{*\top}. \quad (5)$$

Above, we performed the change of variables $S = \arctan(\Theta^*)$. This contains an element-wise differential, simple to compute:

$$dS = \Omega d\Theta, \quad (6)$$

where $\Omega_i = 1/(1 + \Theta_i^2)$ is a diagonal matrix and $i = 1, \dots, d$ iterates over the diagonal. Since W^* is an orthogonal matrix, $W^{*\top} dW^*$ is skew-symmetric. This constraint leads to Townsend's solution [2] for equation 5. We use this result and reverse the change of variables to obtain the update equations for each variable:

$$\begin{aligned} \dot{W}^* &= W^*(F \circ [W^{*\top} \dot{H} Z^* \arctan(\Theta^*) \\ &\quad + \arctan(\Theta^*) Z^{*\top} \dot{H}^\top W^*] \\ &\quad + (I - W^* W^{*\top}) \dot{H} Z^* \arctan(\Theta^*)^{-1}). \end{aligned} \quad (7)$$

$$\dot{\Theta}^* = I \circ [W^{*\top} \dot{H} Z^*] \Omega^{-1} \quad (8)$$

$$\begin{aligned} \dot{Z}^* &= Z^*(F \circ [\arctan(\Theta^*) W^{*\top} \dot{H} Z^* \\ &\quad + Z^{*\top} \dot{H}^\top W^* \arctan(\Theta^*)]) \\ &\quad + (I - Z^* Z^{*\top}) \dot{H}^\top W^* \arctan(\Theta^*)^{-1}. \end{aligned} \quad (9)$$

\circ represents the Hadamard product, and I represents the identity matrix. F is a matrix of the form:

$$F_{ij} = \begin{cases} 1/(\arctan^2(\Theta_j) - \arctan^2(\Theta_i)), & i \neq j \\ 0, & i = j. \end{cases} \quad (10)$$

The results \dot{W}^* , $\dot{\Theta}^*$ and \dot{Z}^* are m -leftmost matrices, so to continue back to the full matrix gradients we can fill in columns of zeros until the matrices become square, where then we write then as \dot{W} , $\dot{\Theta}$ and \dot{Z} . Then, the next step is to consider the equation $W\Theta Z^\top = B^\top$. Since it is a reconstruction rather than a decomposition, its update equation can be obtained as:

$$\begin{aligned} \dot{B}^\top &= [W(F \circ [W^\top \dot{W} - \dot{W}^\top W])\Theta \\ &\quad + (I - WW^\top) \dot{W} \Theta^{-1}] Z^\top \\ &\quad + W(I \circ \dot{\Theta}) Z^\top + W[\Theta(F \circ [Z^\top \dot{Z} - \dot{Z}^\top Z]) Z^\top \\ &\quad + \Theta^{-1} \dot{Z}^\top (I - ZZ^\top)], \end{aligned} \quad (11)$$

where F follows equation 10, but the non-diagonals are defined as $1/(\Theta_j^2 - \Theta_i^2)$.

Finally we consider the equation $B^\top = (\mathbf{X}^\top \mathbf{K})^{-1}(\mathbf{X}^\top - \mathbf{X}^\top \mathbf{K} \mathbf{K}^\top)$. We transpose it and call $A = (\mathbf{X}^\top - \mathbf{X}^\top \mathbf{K} \mathbf{K}^\top)$ and $C = (\mathbf{X}^\top \mathbf{K})^{-1}$, then derivate it by the product rule, massaging the equation to obtain a general form:

$$d\mathbf{B} = d\mathbf{A}C + \mathbf{A}dC \quad (12)$$

$$d\mathbf{A} = d\mathbf{X} - (d\mathbf{K} \mathbf{K}^\top \mathbf{X} + \mathbf{K} d\mathbf{K}^\top \mathbf{X} + \mathbf{K} \mathbf{K}^\top d\mathbf{X}) \quad (13)$$

$$dC = -(\mathbf{K}^\top \mathbf{X})^{-1}(d\mathbf{K}^\top \mathbf{X} + \mathbf{K}^\top d\mathbf{X})(\mathbf{K}^\top \mathbf{X})^{-1} \quad (14)$$

We obtain two update rules, one to from $d\mathbf{B}$ with respect to \mathbf{X} in case a gradient-based pre-processing needs it, and one with respect to \mathbf{K} to update it as a parameter. The derivative with respect to \mathbf{X} is calculated as follows. First we consider $d\mathbf{K} = 0$:

$$\begin{aligned} d\mathbf{B} = & (\mathbf{X} - (d\mathbf{K} \mathbf{K}^\top \mathbf{X} + \mathbf{K} d\mathbf{K}^\top \mathbf{X} \\ & + \mathbf{K} \mathbf{K}^\top d\mathbf{X}))C + \mathbf{A}(-(\mathbf{K}^\top \mathbf{X})^{-1}(d\mathbf{K}^\top \mathbf{X} \\ & + \mathbf{K}^\top d\mathbf{X} + \mathbf{K}^\top d\mathbf{X})(\mathbf{K}^\top \mathbf{X})^{-1}) \end{aligned} \quad (15)$$

$$\begin{aligned} d\mathbf{B} = & (\mathbf{I} - \mathbf{K} \mathbf{K}^\top)d\mathbf{X}(\mathbf{K}^\top \mathbf{X})^{-1} \\ & - \mathbf{A}(\mathbf{K}^\top \mathbf{X})^{-1}\mathbf{K}^\top d\mathbf{X}(\mathbf{K}^\top \mathbf{X})^{-1} \end{aligned} \quad (16)$$

$$d\mathbf{B} = (\mathbf{I} - \mathbf{K} \mathbf{K}^\top - \mathbf{A}(\mathbf{K}^\top \mathbf{X})^{-1}\mathbf{K}^\top)d\mathbf{X}(\mathbf{K}^\top \mathbf{X})^{-1} \quad (17)$$

Then, since our loss function outputs a single real value, we can massage the equations to a canonical form $dL = \text{tr} \dot{\mathbf{B}}^\top d\mathbf{B}$:

$$\begin{aligned} dL = \text{tr} \dot{\mathbf{B}}^\top & ((\mathbf{I} - \mathbf{K} \mathbf{K}^\top \\ & - \mathbf{A}(\mathbf{K}^\top \mathbf{X})^{-1}\mathbf{K}^\top)d\mathbf{X}(\mathbf{K}^\top \mathbf{X})^{-1}), \end{aligned} \quad (18)$$

which leads to the final update equation for the gradient of \mathbf{X} :

$$\dot{\mathbf{X}} = (\mathbf{K}^\top \mathbf{X})^{-1} \dot{\mathbf{B}}^\top [(\mathbf{I} - \mathbf{K} \mathbf{K}^\top)(\mathbf{I} - \mathbf{X}(\mathbf{K}^\top \mathbf{X})^{-1}\mathbf{K}^\top)]. \quad (19)$$

Repeating the same technique, the update equation for \mathbf{K} can be derived as:

$$\begin{aligned} \dot{\mathbf{K}} = & -(\mathbf{K}^\top \mathbf{X})^{-1} \dot{\mathbf{B}}^\top [\mathbf{K}^\top \mathbf{X} \\ & + \mathbf{K}^\top \mathbf{X}^\top + (\mathbf{X}^\top \mathbf{K})^{-1} \mathbf{X}^\top (\mathbf{I} - \mathbf{K} \mathbf{K}^\top)]. \end{aligned} \quad (20)$$

References

- [1] Thomas P Minka. Old and new matrix algebra useful for statistics. See www.stat.cmu.edu/minka/papers/matrix.html, 2000. 1
- [2] James Townsend. Differentiating the singular value decomposition, 2016. 1