Derivative of scalar function w.r.t. matrix arguments

Kadulin V.

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Let $A \in \mathbb{R}^{N \times D}$, $B \in \mathbb{R}^{D \times M}$, $f : \mathbb{R}^{N \times M} \to \mathbb{R}$ is a differentiable function, $C = AB$, $f(C) = y$. We also know $\frac{\partial y}{\partial C}$.

Derive $\frac{\partial y}{\partial A}$, $\frac{\partial y}{\partial B}$.

Let's make a simple example: $N = D = M = 2$. Then

$$A = \begin{bmatrix} a_0 & a_1 \\ a_2 & a_3 \end{bmatrix}, B = \begin{bmatrix} b_0 & b_1 \\ b_2 & b_3 \end{bmatrix}, C = \begin{bmatrix} c_0 & c_1 \\ c_2 & c_3 \end{bmatrix}.$$

1 $\frac{\partial y}{\partial A}$

1. Let's consider first row of $A = a$ and first column of $B = b$. Then $c_0 = a \cdot b = a_0 b_0 + a_1 b_2$ is a scalar.

$$\frac{\partial y}{\partial a_0} = \frac{\partial y}{\partial c_0} \frac{\partial c_0}{\partial a_0} = \frac{\partial y}{\partial c_0} b_0$$

2. Let's consider first row of $A = a$ and full matrix B. Then $c = aB = \begin{bmatrix} c_0 & c_1 \end{bmatrix} = \begin{bmatrix} a_0 b_0 + a_1 b_2 & a_0 b_1 + a_1 b_3 \end{bmatrix}$ is a row vector.

$$\frac{\partial y}{\partial a_0} = \frac{\partial y}{\partial c} \frac{\partial c}{\partial a_0} = \begin{bmatrix} \frac{\partial y}{\partial c_0} & \frac{\partial y}{\partial c_1} \end{bmatrix} \begin{bmatrix} b_0 & b_1 \end{bmatrix}^\top$$

Note that:

- left operand is i-th row in $\frac{\partial y}{\partial C}$, $0 \leq i < N$
- right operand is transposed j-th row in B, $0 \leq j < D$

So, $\frac{\partial y}{\partial A} = \frac{\partial y}{\partial C} B^\top$.

2 $\frac{\partial y}{\partial B}$

1. Let's consider first row of $A = a$ and first column of $B = b$. Then $c_0 = a \cdot b = a_0 b_0 + a_1 b_2$ is a scalar.

$$\frac{\partial y}{\partial b_0} = \frac{\partial y}{\partial c_0} \frac{\partial c_0}{\partial b_0} = \frac{\partial y}{\partial c_0} a_0$$

2. Let's consider full matrix A and first column of $B = b$. Then $c = Ab = \begin{bmatrix} c_0 \\ c_2 \end{bmatrix} = \begin{bmatrix} a_0 b_0 + a_1 b_2 \\ a_2 b_0 + a_3 b_2 \end{bmatrix}$ is a column vector.

$$\frac{\partial y}{\partial b_0} = \frac{\partial y}{\partial c} \frac{\partial c}{\partial b_0} = \begin{bmatrix} \frac{\partial y}{\partial c_0} \\ \frac{\partial y}{\partial c_2} \end{bmatrix}^\top \begin{bmatrix} a_0 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_0 \\ a_2 \end{bmatrix}^\top \begin{bmatrix} \frac{\partial y}{\partial c_0} \\ \frac{\partial y}{\partial c_2} \end{bmatrix}$$

Note that:

- left operand is transposed i-th column in A, $0 \leq i < D$
- right operand is j-th column in $\frac{\partial y}{\partial C}$, $0 \leq j < M$

So, $\frac{\partial y}{\partial B} = A^\top \frac{\partial y}{\partial C}$.