ML Pairwise Distance Function

This document will explain how to calculate pairwise distance between X and Y without needing a third dimension.

Imagine we have $N = 3$, $M = 4$, $D = 2$ and

$$X_{3\times 2} = \begin{bmatrix} 1 & 5 \\ 2 & 3 \\ 4 & 5 \end{bmatrix}, \; Y_{4\times 2} = \begin{bmatrix} 3 & 4 \\ 2 & 5 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}$$

How do we execute $Z^2 = (X - Y)^2$ without needing a third dimension? Consider how the math from the 3D case can be simplified to eliminate that D dimension from the beginning. Feel free to skip to page 3 if you already understand the 3D case.

First, let's examine the slow solution of broadcasting X and Y through 3 dimensions to solve for Z^2. (Note: you can interpret the 3D case as a list of matrices for ease of use)

$$X_{3\times 1\times 2} = \begin{bmatrix}\begin{bmatrix} 1 & 5 \end{bmatrix}, \begin{bmatrix} 2 & 3 \end{bmatrix}, \begin{bmatrix} 4 & 5 \end{bmatrix}\end{bmatrix}$$

$$Y_{1\times 4\times 2} = \begin{bmatrix}\begin{bmatrix} 3 & 4 \\ 2 & 5 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}\end{bmatrix}$$

$$X_{3\times 4\times 2} = \begin{bmatrix}\begin{bmatrix} 1 & 5 \\ 1 & 5 \\ 1 & 5 \\ 1 & 5 \end{bmatrix}, \begin{bmatrix} 2 & 3 \\ 2 & 3 \\ 2 & 3 \\ 2 & 3 \end{bmatrix}, \begin{bmatrix} 4 & 5 \\ 4 & 5 \\ 4 & 5 \\ 4 & 5 \end{bmatrix}\end{bmatrix}$$

$$Y_{3\times 4\times 2} = \begin{bmatrix}\begin{bmatrix} 3 & 4 \\ 2 & 5 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}, \begin{bmatrix} 3 & 4 \\ 2 & 5 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}, \begin{bmatrix} 3 & 4 \\ 2 & 5 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}\end{bmatrix}$$

Now, I'll compute X-Y.

$$(X-Y) = \begin{bmatrix} \begin{bmatrix} 1-3 & 5-4 \\ 1-2 & 5-5 \\ 1-1 & 5-2 \\ 1-3 & 5-2 \end{bmatrix}, \begin{bmatrix} 2-3 & 3-4 \\ 2-2 & 3-5 \\ 2-1 & 3-2 \\ 2-3 & 3-2 \end{bmatrix}, \begin{bmatrix} 4-3 & 5-4 \\ 4-2 & 5-5 \\ 4-1 & 5-2 \\ 4-3 & 5-2 \end{bmatrix} \end{bmatrix}$$

$$(X-Y) = \begin{bmatrix} \begin{bmatrix} -2 & 1 \\ -1 & 0 \\ 0 & 3 \\ -2 & 3 \end{bmatrix}, \begin{bmatrix} -1 & -1 \\ 0 & -2 \\ 1 & 1 \\ -1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 2 & 0 \\ 3 & 3 \\ 1 & 3 \end{bmatrix} \end{bmatrix}$$

$$Z^2_{3x4x2} = (X-Y)^2 = \begin{bmatrix} \begin{bmatrix} 4 & 1 \\ 1 & 0 \\ 0 & 9 \\ 4 & 9 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 0 & 4 \\ 1 & 1 \\ 1 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 4 & 0 \\ 9 & 9 \\ 1 & 9 \end{bmatrix} \end{bmatrix}$$

Now we can sum across D. Then we can rewrite in 2 dimensions.

$$Z^2_{3\times4\times1} = \begin{bmatrix} \begin{bmatrix} 5 \\ 1 \\ 9 \\ 13 \end{bmatrix}, \begin{bmatrix} 2 \\ 4 \\ 2 \\ 2 \end{bmatrix}, \begin{bmatrix} 2 \\ 4 \\ 18 \\ 10 \end{bmatrix} \end{bmatrix}$$

$$Z^2_{3\times4} = \begin{bmatrix} 5 & 1 & 9 & 13 \\ 2 & 4 & 2 & 2 \\ 2 & 4 & 18 & 10 \end{bmatrix}$$

Note: You still have to compute Z which is the square root of the above matrix. But that's easy and irrelevant to the optimization step.

Now I've demonstrated how to calculate Z^2 using three dimensions. But let's examine the end result in terms of the original inputs throughout all the math. (Note: the notation $X_{i,:}$ denotes all the elements within the ith row of X, so $X_{1,:} = [1 \quad 5]$. I'm also going to switch to representing 3 dimensions as a matrix of lists, where a matrix with dimension NxMxD will have N rows, M columns, and D denotes the complexity of each element in the matrix which is a list of size D).

$$(X - Y)_{3x4x2} = \begin{bmatrix} X_{1,:} - Y_{1,:} & X_{1,:} - Y_{2,:} & X_{1,:} - Y_{3,:} & X_{1,:} - Y_{4,:} \\ X_{2,:} - Y_{1,:} & X_{2,:} - Y_{2,:} & X_{2,:} - Y_{3,:} & X_{2,:} - Y_{4,:} \\ X_{3,:} - Y_{1,:} & X_{3,:} - Y_{2,:} & X_{3,:} - Y_{3,:} & X_{3,:} - Y_{4,:} \end{bmatrix}$$

This is the matrix that was shown before for expressing $(X - Y)$, which is obviously 3D. Let's take only the first element of the matrix and express it as w for a moment.

$$w = X_{1,:} - Y_{1,:} = [1 \quad 5] \; - \; [3 \quad 4] = [-2 \quad 1]$$

We can see $(X - Y)$ is 3D because calculating each element of the matrix of $(X - Y)$ is a 1D case. Now how does w eventually transform into the first element of the 2D Z^2 I calculated at the end of page 2? It's just the sum of squares (note: $Z^2_{i,j}$ denotes the element in the ith row of the jth column of Z^2):

$$Z^2_{1,1} = w_1^2 + w_2^2 = (-2)^2 + (1)^2 = 5$$

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Now let's express $Z^2_{1,1}$ in terms of the original inputs.

$$Z^2_{1,1} = (X_{1,1} - Y_{1,1})^2 + (X_{1,2} - Y_{1,2})^2 = (1 - 3)^2 + (5 - 4)^2 = 5$$

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How do we generalize for any element of Z^2?

$$Z^2_{i,j} = (X_{i,1} - Y_{j,1})^2 + (X_{i,2} - Y_{j,2})^2$$

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Finally, let's generalize for any possible dimension D.

$$Z^2_{i,j} = \sum_{d}^{D} (X_{i,d} - Y_{j,d})^2$$

We now have a general closed form for calculating Z^2! But if we go and implement this, it's obviously going to need a third dimension.

So how can we solve for $Z^2_{i,j}$ without needing the third dimension? Let's use the hint of expanding $(X - Y)^2$. (Note: $\cdot$ indicates a dot multiplication).

$$\sum_d^D (X_{i,d} - Y_{j,d})^2 = \sum_d^D X^2_{i,d} - 2 * X_{i,d} \cdot Y_{j,d} + Y^2_{j,d}$$

What in the hell does this mess mean? Let's use our old friend $Z^2_{1,1}$ to understand it better.

$$\begin{aligned}
Z^2_{1,1} = \sum_d^D (X_{1,d} - Y_{1,d})^2 &= \sum_d^D X^2_{1,d} - 2 * X_{1,d} \cdot Y_{1,d} + Y^2_{1,d} \\
&= \sum_d^D [1^2 \quad 5^2] - 2 * [1 \quad 5] \cdot [3 \quad 4] + [3^2 \quad 4^2] \\
&= \sum_d^D [1 \quad 25] - 2 * (1 * 3 + 5 * 4) + [9 \quad 16] \\
&= \sum_d^D [1 \quad 25] - 46 + [9 \quad 16] \\
&= 26 - 46 + 25 = 5
\end{aligned}$$

Now here's a question, did this require a third dimension? In other words, could we have summed over D before recombining the matrices, such that calculating every element in Z^2 doesn't require that D dimension? Intuitively speaking, if you're able to deal with $\sum_d^D$ before dealing with $(X_{i,d} - Y_{j,d})^2$ by expanding as shown above, then the third dimension is unneeded.