Calculating the gradient of a cosine similarity loss function

With v, w vectors, the cosine similarity is defined as

$$sim\left(x, y\right) \frac{v \cdot w}{\sqrt{v \cdot v * w \cdot w}}$$

Now with a matrix transformation $v = Mx$, $w = My$, we have a cosine similarity of

$$sim(x, y, M) = \frac{My \cdot Mx}{\sqrt{Mx \cdot Mx * My \cdot My}}$$

We want to calculate the derivatives wrt M. First we note

$$\frac{\partial v_k}{\partial M_{ij}} = \delta_{ik} x_j$$
$$\frac{\partial w_k}{\partial M_{ij}} = \delta_{ik} y_j$$

$$\frac{\partial \left(a \cdot z\right)}{\partial M_{ij}} = \sum_k \frac{\partial a_k}{\partial M_{ij}} z_k + a_k \frac{\partial z_k}{\partial M_{ij}}$$

Applying this, we have

$$\begin{aligned}
\frac{\partial \left(\frac{v \cdot w}{\sqrt{v \cdot v * w \cdot w}}\right)}{\partial M_{ij}} &= \frac{\frac{\partial (v \cdot w)}{\partial M_{ij}}}{\sqrt{v \cdot v * w \cdot w}} - \frac{v \cdot w}{2\left(v \cdot v * w \cdot w\right)^{\frac{3}{2}}} \frac{\partial \left(v \cdot v * w \cdot w\right)}{\partial M_{ij}} \\
&= \frac{\sum_k \delta_{ik} x_j w_k + v_k \delta_{ik} y_j}{\sqrt{v \cdot v * w \cdot w}} - \frac{v \cdot w}{2\left(v \cdot v * w \cdot w\right)^{\frac{3}{2}}} \left(\sum_k 2\delta_{ik} x_j v_k * w \cdot w + v \cdot v * \sum_k 2\delta_{ik} y_j w_k\right) \\
&= \frac{x_j w_i + v_i y_j}{\sqrt{v \cdot v * w \cdot w}} - \frac{v \cdot w}{\left(v \cdot v * w \cdot w\right)^{\frac{3}{2}}} \left(x_j v_i * w \cdot w + v \cdot v * y_j w_i\right) \\
&= \frac{x_j w_i + v_i y_j}{\left(v \cdot v * w \cdot w\right)^{3/2}} \left(v \cdot v * w \cdot w\right) - \frac{v \cdot w}{\left(v \cdot v * w \cdot w\right)^{\frac{3}{2}}} \left(x_j v_i * w \cdot w + v \cdot v * y_j w_i\right) \\
&= \frac{\left(x_j w_i + v_i y_j\right) v \cdot v * w \cdot w - v \cdot w \left(x_j v_i * w \cdot w + v \cdot v * y_j w_i\right)}{\left(v \cdot v * w \cdot w\right)^{3/2}}
\end{aligned}$$

This last formula is the one that is coded

With Normalized vectors

If we normalize x and y before computation, we note this does not change the cosine similarity of the original vectors or the transformed vectors

As a Hermitian Inner Product

We note that

$$\frac{My\cdot Mx}{\sqrt{Mx\cdot Mx * My\cdot My}}=\frac{y^TM^TMx}{\sqrt{x^TM^TMx * y^TM^TMy}}$$

We note that M only shows up in the form M^TM. So we actually don't need to treat M as a transformation, but a normal inner product $A=M^TM$. We note that M^TM will be symmetric for any M. Thus instead of optimizing over M as an arbitrary matrix, we optimize over A as a symmetric matrix, reducing the number of parameters by half. Thus the similarity measure is

$$sim\left(x,y,A\right)=\frac{y^TAx}{\sqrt{x^TAx * y^TAy}}$$

To optimize over A, we need to calculate the derivative of sim wrt the components of A. First we note

$$\frac{\partial a^TAb}{\partial A_{ij}}=a_ib_j$$

$$\begin{aligned}
\frac{\partial sim}{\partial A_{ij}} &= \frac{y_ix_j}{\sqrt{x^TAx * y^TAy}}-\frac{y^TAx}{2\left(x^TAx * y^TAy\right)^{\left(\frac{3}{2}\right)}}\left(x_ix_jy^TAy+x^TAxy_iy_j\right)\\
&= \frac{2y_ix_j\left(x^TAx * y^TAy\right)-y^TAx\left(x_ix_jy^TAy+x^TAxy_iy_j\right)}{2\left(x^TAx * y^TAy\right)^{\left(\frac{3}{2}\right)}}\\
&= \frac{2y_ix_j\left(x^TAx * y^TAy\right)-y^TAx\left(x_ix_jy^TAy+x^TAxy_iy_j\right)}{2\left(x^TAx * y^TAy\right)^{\left(\frac{3}{2}\right)}}
\end{aligned}$$

We can simplify this calculation by defining $n=x^TAx$, $m=y^TAy$, $l=x^TAy$. Yielding

$$sim\left(x,y,A\right)=\frac{l}{\sqrt{nm}}$$

$$\frac{\partial sim}{\partial A_{ij}}=\frac{2y_ix_jnm-lmx_ix_j-lny_iy_j}{2\left(nm\right)^{\left(\frac{3}{2}\right)}}$$

If we consider the fact that the parameters A_{ij} and A_{ji} are tied together, we can calculate a total gradient for the off-diagonal elements of

$$\frac{dsim}{dA_{ij}}=\frac{2\left(y_ix_j+y_jx_i\right)nm-2lmx_ix_j-2lny_iy_j}{2\left(nm\right)^{\left(\frac{3}{2}\right)}}=\frac{\left(y_ix_j+y_jx_i\right)nm-lmx_ix_j-lny_iy_j}{\left(nm\right)^{\left(\frac{3}{2}\right)}}$$

And for the on-diagonal elements, we get

$$\frac{dsim}{dA_{ii}} = \frac{2y_i x_i nm - lmx_i^2 - lny_i^2}{2\,(nm)^{\left(\frac{3}{2}\right)}}$$