Supplemental Material

A Proof of proposition 1

Let $\langle \boldsymbol{K}^X \rangle_i = \frac{1}{M} \sum_j \boldsymbol{K}^X_{ij}$ denote the average of row i in $\boldsymbol{K}^X$. Likewise, let $\langle \boldsymbol{D}^X \rangle_i = \frac{1}{M} \sum_j \boldsymbol{D}^X_{ij}$ denote the average of row i in $\boldsymbol{D}^X$. By symmetry, note that $\langle \boldsymbol{K}^X \rangle_i$ and $\langle \boldsymbol{D}^X \rangle_i$ are also equal to the average of column i in $\boldsymbol{K}^X$ and $\boldsymbol{D}^X$, respectively. Additionally, let $\langle\!\langle \boldsymbol{K}^X \rangle\!\rangle = \frac{1}{M^2} \sum_{ij} \boldsymbol{K}^X_{ij}$ denote the average element of $\boldsymbol{K}^X$. Likewise, let $\langle\!\langle \boldsymbol{D}^X \rangle\!\rangle = \frac{1}{M^2} \sum_{ij} \boldsymbol{D}^X_{ij}$ denote the average element of $\boldsymbol{D}^X$. Finally, we write the elements of the $M \times M$ centering matrix as $\boldsymbol{C}_{ij} = \delta_{ij} - \frac{1}{M}$, where $\delta_{ij} = 1$ if $i = j$ and equal to zero otherwise (i.e. the Kronecker delta function).

Using this notation, we can write the elements of the centered RDM as:

$$
\begin{aligned}
[\boldsymbol{C}\boldsymbol{D}^X\boldsymbol{C}]_{ij} &= \sum_{k\ell} \boldsymbol{C}_{ik} \boldsymbol{D}^X_{k\ell} \boldsymbol{C}_{\ell j} && (17) \\
&= \sum_{k\ell} (\delta_{ik} - \tfrac{1}{M}) \boldsymbol{D}^X_{k\ell} (\delta_{\ell j} - \tfrac{1}{M}) && (18) \\
&= \sum_{k\ell} \delta_{ik}\delta_{\ell j} \boldsymbol{D}^X_{k\ell} - \frac{1}{M} \sum_{k\ell} \delta_{ik} \boldsymbol{D}^X_{k\ell} - \frac{1}{M} \sum_{k\ell} \delta_{\ell j} \boldsymbol{D}^X_{k\ell} + \frac{1}{M^2} \sum_{k\ell} \boldsymbol{D}^X_{k\ell} && (19) \\
&= \boldsymbol{D}^X_{ij} - \langle \boldsymbol{D}^X \rangle_i - \langle \boldsymbol{D}^X \rangle_j + \langle\!\langle \boldsymbol{D}^X \rangle\!\rangle && (20)
\end{aligned}
$$

Using identical algebriac manipulations, we see that the centered kernel matrix is given by:

$$
[\boldsymbol{C}\boldsymbol{K}^X\boldsymbol{C}]_{ij} = \boldsymbol{K}^X_{ij} - \langle \boldsymbol{K}^X \rangle_i - \langle \boldsymbol{K}^X \rangle_j + \langle\!\langle \boldsymbol{K}^X \rangle\!\rangle \tag{21}
$$

Now substitute in the definition of the RDM in terms of the the kernel matrix to achieve the following set of relations:

$$
\begin{aligned}
\boldsymbol{D}^X_{ij} &= \boldsymbol{K}^X_{ii} + \boldsymbol{K}^X_{jj} - 2\boldsymbol{K}^X_{ij} && (22) \\
\langle \boldsymbol{D}^X \rangle_i &= \boldsymbol{K}^X_{ii} + \frac{1}{M} \operatorname{Tr}[\boldsymbol{K}^X] - 2\langle \boldsymbol{K}^X \rangle_i && (23) \\
\langle \boldsymbol{D}^X \rangle_j &= \frac{1}{M} \operatorname{Tr}[\boldsymbol{K}^X] + \boldsymbol{K}^X_{jj} - 2\langle \boldsymbol{K}^X \rangle_j && (24) \\
\langle\!\langle \boldsymbol{D}^X \rangle\!\rangle &= \frac{2}{M} \operatorname{Tr}[\boldsymbol{K}^X] - 2\langle\!\langle \boldsymbol{K}^X \rangle\!\rangle && (25)
\end{aligned}
$$

Plugging these four relationships into eq. (20) and simplifying yields:

$$
[\boldsymbol{C}\boldsymbol{D}^X\boldsymbol{C}]_{ij} = -2\boldsymbol{K}^X_{ij} + 2\langle \boldsymbol{K}^X \rangle_i + 2\langle \boldsymbol{K}^X \rangle_j - 2\langle\!\langle \boldsymbol{K}^X \rangle\!\rangle = -2[\boldsymbol{C}\boldsymbol{K}^X\boldsymbol{C}]_{ij} \tag{26}
$$

Thus, the centered RDM is equal to negative two times the centered kernel matrix. The proposition then immediately follows by recognizing that the cosine similarity function, defined in eq. (1), is invariant to this rescaling. That is, for any $c \neq 0$ and any symmetric matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ we have:

$$
S(c\boldsymbol{A}, c\boldsymbol{B}) = \frac{\operatorname{Tr}[c^2 \boldsymbol{A}\boldsymbol{B}]}{\|c\boldsymbol{A}\|_F \|c\boldsymbol{B}\|_F} = \frac{c^2}{|c| \cdot |c|} S(\boldsymbol{A}, \boldsymbol{B}) = S(\boldsymbol{A}, \boldsymbol{B}) \tag{27}
$$

Thus, we have:

$$
S(\boldsymbol{C}\boldsymbol{D}^X\boldsymbol{C}, \boldsymbol{C}\boldsymbol{D}^Y\boldsymbol{C}) = S(-2 \cdot \boldsymbol{C}\boldsymbol{K}^X\boldsymbol{C}, -2 \cdot \boldsymbol{C}\boldsymbol{K}^Y\boldsymbol{C}) = S(\boldsymbol{C}\boldsymbol{K}^X\boldsymbol{C}, \boldsymbol{C}\boldsymbol{K}^Y\boldsymbol{C}) \tag{28}
$$

as claimed by the proposition.