Properties of the Trace

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The trace $\mathrm{tr}(\boldsymbol{A})$ of a square matrix $\boldsymbol{A} \in \mathbb{R}^{D \times D}$ is the defined as the sum of the diagonal elements, i.e.,

$$\mathrm{tr}(\boldsymbol{A}) = \sum_{d=1}^{D} A_{dd}, \quad \boldsymbol{A} \in \mathbb{R}^{D \times D}. \tag{1}$$

It has the following properties:

$$\mathrm{tr}(\alpha) = \alpha, \quad \alpha \in \mathbb{R} \tag{2}$$

$$\mathrm{tr}(\boldsymbol{A} + \boldsymbol{B}) = \mathrm{tr}(\boldsymbol{A}) + \mathrm{tr}(\boldsymbol{B}), \quad \boldsymbol{A}, \boldsymbol{B} \in \mathbb{R}^{D \times D} \tag{3}$$

$$\mathrm{tr}(\boldsymbol{ABC}) = \mathrm{tr}(\boldsymbol{BCA}) = \mathrm{tr}(\boldsymbol{CAB}), \quad \boldsymbol{A} \in \mathbb{R}^{D \times E}, \boldsymbol{B} \in \mathbb{R}^{E \times F}, \boldsymbol{C} \in \mathbb{R}^{F \times D} \tag{4}$$

Exploiting these properties (jumping toward the end of the PCA loss function reformulation [1]), we get

$$\begin{aligned}
\sum_{j=M+1}^{D} \underbrace{\boldsymbol{b}_j^\top \boldsymbol{S} \boldsymbol{b}_j}_{\in \mathbb{R}} &\overset{(2)}{=} \sum_{j=M+1}^{D} \mathrm{tr}(\boldsymbol{b}_j^\top \boldsymbol{S} \boldsymbol{b}_j) && (5)\\
&\overset{(4)}{=} \sum_{j=M+1}^{D} \mathrm{tr}(\boldsymbol{S} \boldsymbol{b}_j \boldsymbol{b}_j^\top) && (6)\\
&\overset{(4)}{=} \sum_{j=M+1}^{D} \mathrm{tr}(\boldsymbol{b}_j \boldsymbol{b}_j^\top \boldsymbol{S}) && (7)\\
&\overset{(3)}{=} \mathrm{tr}\left(\sum_{j=M+1}^{D} \boldsymbol{b}_j \boldsymbol{b}_j^\top \boldsymbol{S} \right) && (8)\\
&= \mathrm{tr}\left(\Big(\sum_{j=M+1}^{D} \boldsymbol{b}_j \boldsymbol{b}_j^\top \Big) \boldsymbol{S} \right) && (9)
\end{aligned}$$

where in the last step we used the fact that $\boldsymbol{S}$ is independent of j, so that we could move it out of the sum. For further details on the trace and the reformulation of the loss function in PCA, we refer to [1], Chapter 10.3.

References

[1] M. P. Deisenroth, A. A. Faisal, and C. S. Ong. *Mathematics for Machine Learning*. Cambridge University Press, 2020.