A NOTE ON THE RELATIONSHIP BETWEEN PCA AND SVD

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We assume that we are calculating over the field of real numbers, denoted by $\mathbb{R}$. In this case, the *singular value decomposition* (SVD) of an $m \times n$ matrix M is defined as

$$M = U\Sigma V^{\intercal}, \tag{1}$$

where U is an $m \times m$ orthogonal matrix, Σ is a diagonal $m \times n$ matrix with non-negative real numbers (the *singular values*) on the diagonal, and $V^{\intercal}$ is the transpose of an $n \times n$ orthogonal matrix. Note that the SVD of M *always* exists, regardless of the other properties of the matrix M. In particular, this factorization is well-defined for 'degenerate' matrices with more columns than rows. Its calculation has a complexity of $\mathcal{O}\left(mn^2\right)$.

If we want to calculate a *principal component analysis* (PCA) of M, we usually first calculate the covariance matrix $M^{\intercal}M$. This matrix is by construction symmetric and real-valued, so an eigendecomposition is guaranteed to exist. Similarly, an SVD of this matrix exists, and we have

$$M^{\intercal}M = (U\Sigma V^{\intercal})^{\intercal}(U\Sigma V^{\intercal}) \tag{2}$$

$$= V\Sigma U^{\intercal}U\Sigma V^{\intercal} \tag{3}$$

Since U is orthogonal, we have $U^{\intercal}U = \mathbb{I}$, i.e. the identity matrix, so the previous equation can be simplified and we obtain

$$= V\Sigma^2 V^{\intercal}. \tag{4}$$

This constitutes an eigendecomposition (by orthogonal matrices) of $M^{\intercal}M$ by definition. As Σ^2 is a diagonal $n \times n$ matrix, we can see that the eigenvalues of the PCA decomposition are just the squares of the singular values of the singular value decomposition. Likewise, we can see that the eigenvectors of the PCA decomposition are the singular vectors of the SVD. It is thus possible to calculate a PCA using an SVD.

As the eigendecomposition has a complexity of $\mathcal{O}\left(n^3\right)$, the SVD is generally faster in practice. Moreover, it does not involve calculating the covariance matrix, which makes the SVD numerically more stable.