Data Whitening and Transformation (for uncertainty set specification)

“Data whitening” is the process of transforming a dataset ($M \in \mathbb{R}^{nxm}$) of n features and m observations such that the features are uncorrelated, and each feature has unit variance. In other words, the covariance matrix of the transformed data set is the identity matrix I^{nxn}.

For a centered dataset (mean of each feature is 0) the covariance can be estimated as:

$$\Sigma_M = \frac{MM^T}{m}$$

It follows that:

$$Y = WM$$
$$\Sigma_Y = \frac{YY^T}{m} = \frac{(WM)(WM)^T}{m} = \frac{WMM^TW^T}{m} = W\Sigma_M W^T = I$$

Terms can be grouped and the fact that inverses are commutative ($AA^{-1} = A^{-1}A = I$) can be used to rearrange the equality as follows:

$$I = W(\Sigma_M W^T) = \Sigma_M W^T W$$
$$W^T W = \Sigma_M^{-1}$$

There are many matrices that can make this equality true. It’s clear that the Cholesky decomposition of the inverse covariance matrix works. The square root of the inverse of the covariance matrix works as well:

$$\Sigma_M^{-1/2}\left(\Sigma_M^{-1/2}\right)^T = \Sigma_M^{-1/2}\Sigma_M^{-1/2} = \Sigma_M^{-1}$$

The above equality holds because the inverse square root of a symmetric, positive semidefinite matrix is also symmetric. This can be proved by starting with the proof that the inverse of a symmetric matrix is also symmetric:

If A is symmetric ($A = A^T$) then:

$$AA^{-1} = I = (AA^{-1})^T = (A^{-1})^T A^T = (A^{-1})^T A$$
$$AA^{-1} = A^{-1}A$$
$$A^{-1}AA^{-1} = (A^{-1})^T AA^{-1}$$
$$A^{-1} = (A^{-1})^T$$

Then prove that the inverse of a symmetric PSD matrix is also PSD.

Start with the fact that PSD matrices have positive eigenvalues. If matrix A with eigenvector v is PSD then $v^T A v \geq 0$. *The following logic can then be applied to find that the corresponding eigenvalue must be positive:*

$$v^T A v = v^T \lambda v = \lambda v^T v$$
$$v^T v \geq 0$$
$$\lambda \geq 0$$

Then if λ *is an eigenvalue of* A, $\frac{1}{\lambda}$ *is an eigenvalue for* A^{-1}:

$$Av = \lambda v$$
$$A^{-1}Av = A^{-1}\lambda v = \lambda A^{-1} v = v$$
$$A^{-1}v = \frac{1}{\lambda} v$$

Since the eigenvalues for the symmetric PSD matrix A were all positive, the eigenvalues of A^{-1} *(which is known to be symmetric) are also positive because reciprocals of positive numbers are positive. It follows that* A^{-1} *is symmetric and PSD.*

Finally, prove that the square root of a symmetric PSD matrix is also symmetric.

Let B be a matrix such that $B^2 = A$. *A is a symmetric PSD matrix that can be diagonalized as* $A = Q\Lambda Q^T$ *where Q is orthogonal and* $Q^T Q = I$ *(see proof of orthogonal eigenvectors in symmetric matrices in PSD projection document). Then:*

$$A^{1/2} = Q\Lambda^{1/2}Q^T = Q\begin{bmatrix} \sqrt{\lambda_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sqrt{\lambda_n} \end{bmatrix} Q^T = B$$

Since A is symmetric and PSD, it is known that its eigenvalues are positive, so the square roots of the eigenvalues are real. B has real eigenvalues and it can be diagonalized with orthogonal matrices (the same as A) thus B is symmetric.