Projection of Symmetric Matrix onto the set of Positive Semidefinite (PSD) Matrices

The projection of a point onto a set is defined as the closest point contained in the set to the initial point to be projected. Closest is defined as the Euclidean distance. In the context of this problem, the initial point is the symmetric matrix A and the objective is to find X, a symmetric PSD matrix that is closest to A in the Frobenius norm.

$$\min_X \|A - X\|_2^2$$

Where the Frobenius norm of a matrix M is defined as:

$$\|M\|_2^2 = \sum_{i,j} m_{ij}^2$$

Start with the spectral decomposition for A which is defined below. Λ is the diagonalized matrix of the vector of eigenvalues λ_i. Q is a matrix of eigenvectors where the columns are the corresponding eigenvectors v_i.

$$\begin{gathered} Aq = \lambda q \\ AQ = Q\Lambda \\ AQQ^{-1} = Q\Lambda Q^{-1} \\ A = Q\Lambda Q^{-1} \end{gathered}$$

Then for a symmetric matrix A:

$$A = Q\Lambda Q^T \text{ where } Q^T Q = I$$

In other words, Q is an orthogonal matrix. See proof below.

If $\lambda_1$and $\lambda_2$are eigenvalues of the symmetric matrix A with associated eigenvectors $q_1$and q_2 and $\lambda_1 \neq \lambda_2$then:

$$\begin{gathered} \lambda_1 q_1^T q_2 = q_1^T A^T q_2 = q_1^T A q_2 = q_1^T \lambda_2 q_2 = \lambda_2 q_1^T q_2 \\ \lambda_1 q_1^T q_2 = \lambda_2 q_1^T q_2 \\ (\lambda_1 - \lambda_2) q_1^T q_2 = 0 \end{gathered}$$

It is known that $\lambda_1 \neq \lambda_2$ thus $q_1^T q_2 = 0$. This holds true for every eigenvector pair so then:

$$Q^T Q = \begin{bmatrix} -q_1 - \\ -q_2 - \\ \vdots \\ -q_n - \end{bmatrix} [q_1 \quad q_2 \quad \cdots \quad q_n] = \begin{bmatrix} q_1^T q_1 & 0 & \dots & 0 \\ 0 & q_2^T q_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & q_n^T q_n \end{bmatrix} = I$$

A property of orthogonal matrices is that they have no effect on the Frobenius norm. See proof below:

Given an orthogonal matrix H and another matrix M then:

$$\|HM\|_2^2 = tr(HM(HM)^T) = tr(HMM^TH^T) = tr(H^THMM^T) = \; tr(MM^T) = \|M\|_2^2$$

The third and fourth terms in the equality $tr(HMM^TH^T) = tr(H^THMM^T)$ hold because the trace is invariant to cyclical operations.

$$tr(HM) = \sum_i (HM)_{ii} = \sum_i \sum_j H_{ij}M_{ji} = \sum_j \sum_i M_{ji}H_{ij} = \sum_j (MH)_{jj} = tr(MH)$$

This property is used to transform the inside of the norm:

$$\|A - X\|_2^2 = \|Q\Lambda Q^T - X\|_2^2 = \|Q^T(Q\Lambda Q^T - X)\|_2^2 = \|\Lambda Q^T - Q^TX\|_2^2$$
$$= \|(\Lambda Q^T - Q^TX)Q\|_2^2 = \|\Lambda - Q^TXQ\|_2^2$$

Thus:

$$\min_X \|A - X\|_2^2 = \min_X \|\Lambda - Q^TXQ\|_2^2$$

Let $Y = Q^TXQ$, then:

$$\|\Lambda - Y\|_2^2 \; = \sum_{i \neq j} (y_{ij})^2 + \sum_i (\lambda_{ii} - y_{ii})^2$$

The first term arises from the fact that Λ is diagonal so its elements for when $i \neq j$ are 0. Λ cannot be ignored for the diagonal terms which explains the second term. To minimize the summation, it is clear that $y_{ij} = 0 \; \forall i \neq j$. The second term is minimized when $y_{ii} = \lambda_{ii}$.

It should be noted that A was not PSD to begin with while Y must be PSD. See proof below.

For some matrix M which is positive semidefinite, QMQ^T is PSD if $x^TQMQ^Tx \geq 0 \; \forall x$. It follows that:

$$x^TQMQ^Tx = (Q^Tx)^TM(Q^Tx) \geq 0 \; \forall x$$

This holds true because M itself is PSD and any vector on the "outsides" will result in a value greater than 0.

It then follows that since Y is PSD, its diagonal elements must be greater than or equal to 0. See proof below.

> *For some matrix M that is PSD, $x^T Mx \geq 0\ \forall x$. We know that $x^T Mx = \sum_{i,j} x_i M_{ij} x_j \geq 0$. Then the contribution to the sum from any diagonal element of M is $x_i^2 M_{ii}$. Now we imagine a scenario where $M_{ii} < 0$. In that scenario set x equal to the zero vector except the i-th element. Then $x^T Mx = \sum_{i,j} x_i M_{ij} x_j = x_i^2 M_{ii} < 0\ \forall x_i$. This would force M to not be PSD thus the diagonal must be greater than or equal to 0.*

For the i that $\lambda_{ii} < 0$, $y_{ii} = 0$ minimizes the summation (since $y_{ii} \geq 0$). Y is then:

$$Y = diag(max\{0, \lambda_1\}, max\{0, \lambda_2\}, max\{0, \lambda_3\}, \dots, max\{0, \lambda_n\})$$

It follows that X (the projection of A onto the set of symmetric PSD matrices) is:

$$X = QYQ^T$$