Principal Component Analysis (PCA) and Singular Value Decomposition (SVD)

Consider the following scenario. We measure a signal from a probe surrounded by an unknown number of neurons. We then split the signal into 1 millisecond chunks and sample at about $f_s = 20kH z$. We obtain a graph with the superposition of these neuron pulses.

We now define the following values concerning our signal.

$m \approx 200$ spike traces  
$n = 30$ data points

Each trace occupies a row within the following matrix, $A$.

$$A = \begin{bmatrix} a_1^T \\ \vdots \\ a_m^T \end{bmatrix}_{m \times n}$$

The mean of these traces is as follow:

$$\bar{a}^T = \frac{1}{m} \sum_{l=1}^{m} a_l^T$$

Finally, we create something known as the zero-mean data matrix.

$$x = \begin{bmatrix} x_1^T \\ \vdots \\ x_m^T \end{bmatrix} = \begin{bmatrix} a_1^T - \bar{a}^T \\ \vdots \\ a_m^T - \bar{a}^T \end{bmatrix}$$

Let’s now back up and take a holistic view at what we are trying to do:

(a) Look at the data in the best way.  
(b) Detect patterns in the data.  
(c) Identify key sources of variability.  
(d) Identify and exploit a reduced-dimensional space.
We will first take a look at Singular Value Decomposition (SVD) and then backtrack to Principal Component Analysis (PCA).

Any $m \times n$ matrix $X \in \mathbb{R}^{m \times n}$ can be decomposed as follows:

$$X = U\Sigma V^T$$

$U$ is $m \times m$, $V$ is $n \times n$, and $\Sigma$ is $m \times n$. Moreover, $U$ and $V$ are unitary matrices: $UU^T = U^TU = I_m$ and $VV^T = V^TV = I_n$. Finally $\Sigma$ is a block diagonal matrix. The matrices take the following form:

$$U = \begin{bmatrix}
| & | & | \\
\sigma_1 & \cdots & \sigma_k \\
| & | & | \\
\sigma_k & \cdots & \sigma_m \\
| & | & | \\
\sigma_m & \cdots & \sigma_m \\
| & | & |
\end{bmatrix}$$

$$V = \begin{bmatrix}
| & | & | \\
v_1 & \cdots & v_k \\
| & | & | \\
v_k & \cdots & v_n \\
| & | & | \\
v_n & \cdots & v_n \\
| & | & |
\end{bmatrix}$$

$$\Sigma = \begin{bmatrix}
D & 0 \\
0 & 0
\end{bmatrix}$$

Here, this is noting that both $U$ and $V$ are matrices of column vectors, and $\Sigma$ is a block diagonal matrix with the upper left block being the singular values.

This looks a lot like eigenvalue decomposition for $m \times n$ matrices. The main difference is that in $\Sigma$ instead of eigenvalues, we have singular values of $X$: $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_m$. These values form the main diagonal of $\Sigma$ with the property that they are ordered in decreasing order, i.e. $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_m$.

Proof of Orthogonality for $X$:

$$X^TX = (U\Sigma V^T)^T \Sigma U^T V^T = \Sigma U^T V^T \Sigma = \Sigma^2 V^T$$

The final value in the proof above is symmetric, which shows that $X^TX$ is symmetric, so it must be orthogonal: $X^TX = XX^T$.

Square symmetric matrices have mutually orthogonal eigenvectors corresponding to distinct eigenvalues. $V$ is a matrix of right singular vectors and $U$ is a matrix of left singular vectors. To get $U$, construct $XX^T$ and grab its eigenvector matrix and call it $U$.

Singular vectors are the positive square roots of the eigenvalues of $X^TX$.

The maximum number of nonzero singular values is the minimum of $m$ and $n$. The actual number of positive singular values is $r = \text{rank}(X)$.

Assume that we have a vector $q$, s.t.

$$q^TX^TXq = (Xq^T)(Xq) = ||Xq||^2 \geq 0$$

$$q = \sum \alpha_q v_i \rightarrow q^TX^TXq = \Sigma \geq 0$$
If there is no vector \( q \) where the above statement is true, then all eigenvalues are positive.

Now, we will examine Principal Component Analysis (PCA).

Say that we are after an orthogonal transformation \( V \) to create \( Y \), an \( m \times n \) matrix: \( Y = XV \). We want \( Y \) such that \( Y^T Y \) is diagonal. In essence, we are decorrelating the data.

We define \( V \) such that \( V^T \) is the scaled covariance matrix of original data.

We need to show that if \( Y = XV \) where \( X = UV \), then \( Y^T Y \) is diagonal. We define \( \wedge \) as \( \Sigma^2 \).

\[
Y^T Y = V^T X^T X V = V^T \Sigma^2 V = \wedge
\]

Lecture ends here.