

Machine Learning for Finance (FIN 570) Singular Value Decomposition (SVD) and Principal Component Analysis (PCA)

Instructor: Jaehyuk Choi

Peking University HSBC Business School, Shenzhen, China

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Eigen(spectral) decomposition

For a matrix A , eigenvalue λ_k and eigenvector v_k satisfy

$$Av_k = \lambda_k v_k.$$

The matrix A can be decomposed into

$$A = Q\Lambda Q^{-1},$$

where Λ is a diagonal matrix with values λ_k and $Q = (v_1 \cdots v_n)$, i.e., $Q_{*j} = v_j$.
When A is real and symmetric, Q is an orthonormal matrix, $QQ^T = I$,

$$A = Q\Lambda Q^T,$$

Singular Value Decomposition (SVD)

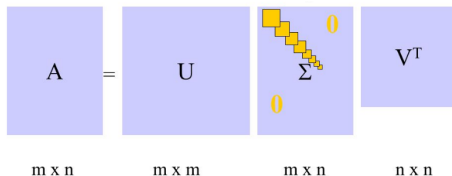
The single most useful practical concept in linear algebra:

- Any matrix (even rectangular) has a SVD.
- SVD tells everything on a matrix.

For any $m \times n$ matrix A , there is a unique decomposition:

$$A = USV^T, \quad \text{where}$$

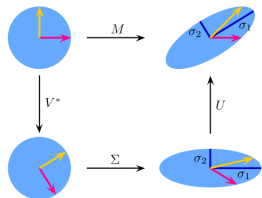
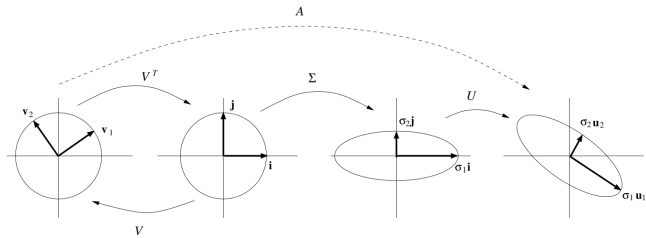
- U ($m \times m$): orthonormal ($UU^T = U^TU = I$)
- S ($m \times n$): diagonal. Singular values, $s_k \geq 0$, are in decreasing order for $1 \leq k \leq \min(m, n)$
- V ($n \times n$): orthonormal ($VV^T = V^TV = I$)



SVD: Intuition

Linear transformation A is decomposed into

- a rotation by V^T
- a scaling by S
- a rotation by U



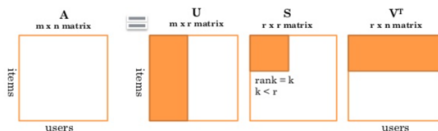
$$M = U \cdot \Sigma \cdot V^*$$

SVD: Compact Form, Low Rank Approximation

$$\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \\ * & * & * \end{bmatrix} = \underbrace{\begin{bmatrix} * & * & * & * \\ * & * & * & * \\ * & * & * & * \\ * & * & * & * \end{bmatrix}}_U \underbrace{\begin{bmatrix} \bullet & & & \\ & \bullet & & \\ & & \bullet & \\ & & & \bullet \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} * & * & * \\ * & * & * \end{bmatrix}}_{V^T}$$

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} = \underbrace{\begin{bmatrix} * & * & * \\ * & * & * \\ * & * & * \end{bmatrix}}_U \underbrace{\begin{bmatrix} \bullet & & & & \\ & \bullet & & & \\ & & \bullet & & \\ & & & \bullet & \\ & & & & \bullet \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix}}_{V^T}$$

$$A = U \times S \times V^T$$

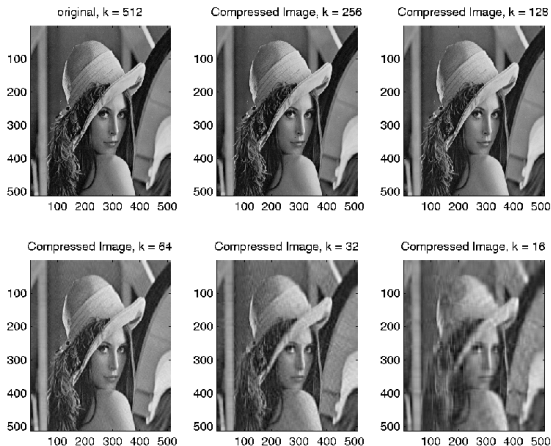


$$A_k = U_k \times S_k \times V_k^T$$

- For a non-square matrix, a compact form is enough:
 U ($m \times r$), S ($r \times r$), V ($n \times r$) where $r = \min(m, n)$.
- If the rank is k ($\leq r$), $s_{j>k} = 0$:
 U ($m \times k$), S ($k \times k$), V ($n \times k$)
- Using the first j ($< k$) biggest singular values,

SVD: Image Compression

An image file is nothing but a matrix, so the low-rank approximation of SVD works as an image compression method. The storage is reduced from mn to $(m + n + 1)k$.



Principal Component Analysis (PCA)

If \mathbf{X} is a matrix of n samples of p features ($n \times p$), the covariance matrix is

$$\Sigma = \frac{1}{n} \mathbf{X}^T \mathbf{X} : (p \times p) \text{ symmetric matrix}$$

The covariance matrix of the transformed space $\mathbf{Z} = \mathbf{X}\mathbf{W}$ is

$$\text{Cov}(\mathbf{Z}) = \frac{1}{n} (\mathbf{X}\mathbf{W})^T (\mathbf{X}\mathbf{W}) = \frac{1}{n} \mathbf{W}^T (\mathbf{X}^T \mathbf{X}) \mathbf{W} = \mathbf{W}^T \Sigma \mathbf{W}$$

If we pick \mathbf{W} to be the orthogonal transformation of SVD , i.e., $\Sigma = \mathbf{W}\mathbf{S}\mathbf{W}^T$,

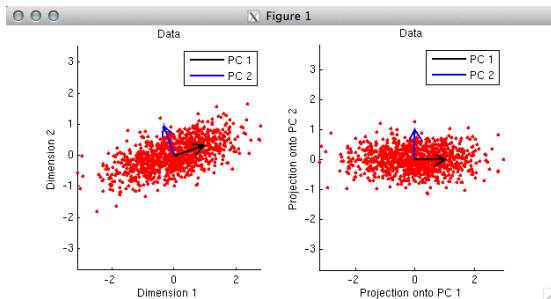
$$\text{Cov}(\mathbf{Z}) = \mathbf{S} = \text{diag}(S_{11}, \dots, S_{pp}).$$

Notice that $\text{Cov}(Z_i, Z_j) = \mathbf{W}_{*i}^T \Sigma \mathbf{W}_{*j} = S_{ij}$ is zero if $i \neq j$, so the extracted features are orthogonal.

Process of finding W

Let $W = (W_{*1} \ W_{*2} \ \cdots \ W_{*p})$.

- Find W_{*1} such that $|W_{*1}| = 1$ and $|W_{*1}^T \Sigma W_{*1}|$ is maximized.
- Find W_{*2} such that $|W_{*2}| = 1$, $|W_{*2}^T \Sigma W_{*2}|$ is maximized and $W_{*1}^T W_{*2} = 0$.
- ...
- Find W_{*k} such that $|W_{*k}| = 1$, $|W_{*k}^T \Sigma W_{*k}|$ is maximized and W_{*k} is orthogonal to $\{W_{*j}\}$ for $j < k$.



Total and Explained Variance

The total variance is the variance of all original features. Under PCA,

$$\sum_{k=1}^p \text{Var}(X_k) = \sum_{k=1}^p S_{kk}.$$

Therefore the ratio

$$\frac{\sum_{j=1}^k S_{jj}}{\sum_{j=1}^p S_{jj}}$$

indicates how much of the total variance is *explained* by the first k PCA factors. Extracting features from PCA is an unsupervised learning, NOT supervised learning, because the response variable is not associated.

PCA vs Simple Linear Regression for (x, y)

PCA is not same as Simple Linear regression (OLS)!

- **Linear Regression** minimize the the (squared) distance in y -axis.
- **PCA** (1st component) minimize the (squared) shortest distance.

