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

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Eigen(spectral) decomposition

For a matrix $\boldsymbol{A}$, eigenvalue λ_k and eigenvector $\boldsymbol{v}_k$ satisfy

$$\boldsymbol{A}\boldsymbol{v}_k = \lambda_k \boldsymbol{v}_k.$$

The matrix $\boldsymbol{A}$ can be decomposed into

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

where $\boldsymbol{\Lambda}$ is a diagonal matrix with values λ_k and $\boldsymbol{Q} = (\boldsymbol{v}_1 \cdots \boldsymbol{v}_n)$, i.e., $\boldsymbol{Q}_{*j} = \boldsymbol{v}_j$.
When $\boldsymbol{A}$ is real and symmetric, $\boldsymbol{Q}$ is an orthogonal matrix, $\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}$,

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^T,$$

Singular Value Decomposition (SVD)

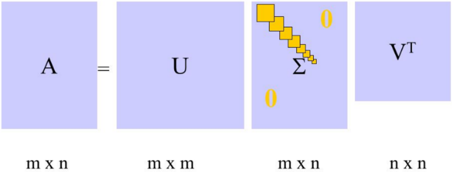
The single most useful practical concept in linear algebra:

- 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:

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

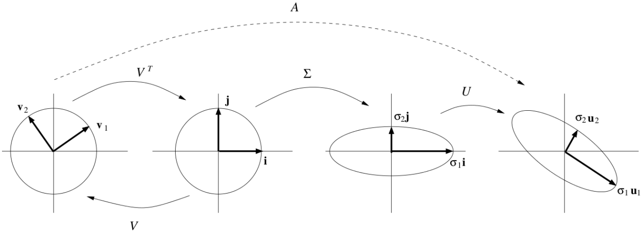
- U $(m \times m)$: orthogonal $(UU^T = U^T U = I)$
- S $(m \times n)$: diagonal. Singular values, $s_k \geq 0$, are in decreasing order for $1 \leq k \leq \min(m, n)$
- V $(n \times n)$: orthogonal $(VV^T = V^T V = I)$

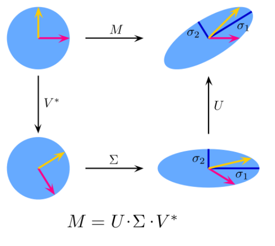


SVD: Intuition

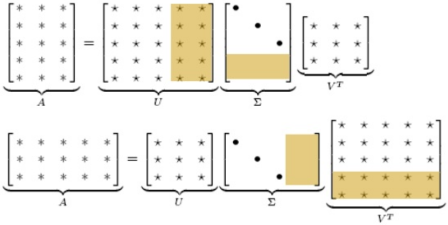
Linear transformation A is decomposed into

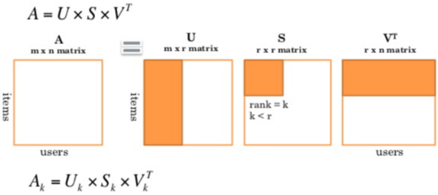
- a rotation by V^T
- a scaling by S
- a rotation by U





SVD: Compact Form, Low Rank Approximation





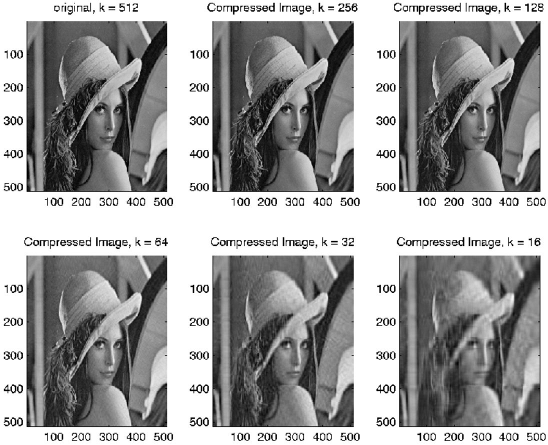
- For a non-square matrix, a compact form is enough: U $(m \times r)$, S $(r \times r)$, V $(n \times r)$ where $r = \min(m, n)$.
- If the rank is k $(\leq r)$, $s_{j>k} = 0$: U $(m \times k)$, S $(k \times k)$, V $(n \times k)$
- Using the first j $(\leq k)$ biggest singular values,

$$A_j = U_j S_j V_j^T = \sum_{i=1}^{j} \boldsymbol{u}_i s_i \boldsymbol{v}_i^T, \quad U_j\,(m \times j),\; S_j\,(j \times j),\; V_j\,(n \times j)$$

is the best approximation with rank j minimizing the norm $\|A - A_j\|_F$

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

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

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

$$\mathrm{Cov}(\boldsymbol{Z}) = \frac{1}{n}(\boldsymbol{XW})^T(\boldsymbol{XW}) = \frac{1}{n}\boldsymbol{W}^T(\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{W} = \boldsymbol{W}^T\Sigma\boldsymbol{W}$$

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

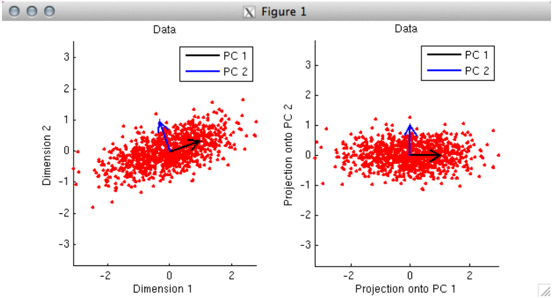
$$\mathrm{Cov}(\boldsymbol{Z}) = \boldsymbol{S} = \mathrm{diag}(S_{11}, \cdots, S_{pp}).$$

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

Process of finding $\boldsymbol{W}$

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

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



Total and Explained Variance

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

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

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.