Linear Systems

Singular Value Decomposition

Sivakumar Balasubramanian

Department of Bioengineering
Christian Medical College, Bagayam
Vellore 632002

Matrices are basis dependent

- Linear transformations represented as matrices depend on the choice of basis. For example, if $\mathbf{A} : \mathbb{R}^n \rightarrow \mathbb{R}^n$represents a linear transformation in the standard basis, then the same transformation in a basis V is given by,

$$\mathbf{V}^{-1}\mathbf{A}\mathbf{V} : \text{Similarity transformation}$$

- In fact, for specific a choice of basis, it is possible to have the simplest possible representation for $\mathbf{A} \longrightarrow$ *Eigen decomposition*.
  When a matrix $\mathbf{A}$ has n eigenpairs $\{(\lambda_i, \mathbf{x}_i)\}_{i=1}^n$, with linearly independent eigenvectors, we have

$$\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$$

- What about rectangular matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$? Can we talk about "similar" matrices in this case?

Matrix equivalence

- Consider a linear transformation $T : \mathbb{R}^n \rightarrow \mathbb{R}^m$, such that $\mathbf{y} = T(\mathbf{x})$, where $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^m$. T can be represented as a matrix $\mathbf{A}$, such that $\mathbf{y} = \mathbf{A}\mathbf{x}$.
- Exact entries of $\mathbf{A}$ will depend on the choice of basis for both the input and the output spaces. Let us assume that the matrix $\mathbf{A}$ is the representation when the standard basis is used for the input and output spaces.
- If a different set of basis are chosen for the input and output spaces, namely $V = \{\mathbf{v}_i\}_{i=1}^n$ $(\mathbf{v}_i \in \mathbb{R}^n)$ and $W = \{\mathbf{w}_i\}_{i=1}^m$ $(\mathbf{w}_i \in \mathbb{R}^m)$. Then the corresponding matrix representation for the linear transformation T is,

$$\mathbf{A}_{VW} = \mathbf{W}^{-1}\mathbf{A}\mathbf{V}$$

  where, the $\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \ldots & \mathbf{v}_n \end{bmatrix}$ and $\mathbf{W} = \begin{bmatrix} \mathbf{w}_1 & \mathbf{w}_2 & \ldots & \mathbf{w}_m \end{bmatrix}$.
- $\mathbf{A}$ and $\mathbf{A}_{VW}$ are called *equivalent matrices*.

Singular Value Decomposition: Diagonalizing any matrix

- Eigen-decomposition provided a way to do this for a square matrix with full rank. $\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$. When $\mathbf{A}$ is symmetric, $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$.
- For rectangular and rank-deficient matrices, we can do this using *singular value decomposition*.
- Consider a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $rank\left(\mathbf{A}\right) = r$.

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \begin{bmatrix}\mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_m\end{bmatrix} \begin{bmatrix}\mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}\end{bmatrix} \begin{bmatrix}\mathbf{v}_1 & \mathbf{v}_2 & \ldots & \mathbf{v}_n\end{bmatrix}^T$$

where, $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{U}\mathbf{U}^T = \mathbf{I}$; $\mathbf{V} \in \mathbb{R}^{n \times n}$, $\mathbf{V}\mathbf{V}^T = \mathbf{I}$; and $\mathbf{D} = \operatorname{diag}\left(\sigma_1 \ldots \sigma_r\right)$.

- Columns $\mathbf{U}$ are eigenvectors of $\mathbf{A}^T\mathbf{A}$, forming an orthonormal basis for $\mathbb{R}^m$.
- Columns $\mathbf{V}$ are eigenvectors of $\mathbf{A}\mathbf{A}^T$, forming an orthonormal basis for $\mathbb{R}^n$.
- $\sigma_i^2 = \lambda_i$, where λ_is are the eigenvalues of $\mathbf{A}^T\mathbf{A}$ and $\mathbf{A}\mathbf{A}^T$.

Singular Value Decomposition: Diagonalizing any matrix

- For $\mathbf{A}$,
$$C(\mathbf{A}) = span\{\hat{\mathbf{u}}_1 \ldots \hat{\mathbf{u}}_r\} \quad N\left(\mathbf{A}^T\right) = span\{\hat{\mathbf{u}}_{r+1} \ldots \hat{\mathbf{u}}_m\}$$
$$C\left(\mathbf{A}^T\right) = span\{\hat{\mathbf{v}}_1 \ldots \hat{\mathbf{v}}_r\} \quad N(\mathbf{A}) = span\{\hat{\mathbf{v}}_{r+1} \ldots \hat{\mathbf{v}}_n\}$$
where, the $\hat{\mathbf{u}}_i$s and the $\hat{\mathbf{v}}_i$s are any orthonormal basis for $\mathbb{R}^m$ and $\mathbb{R}^n$, respectively.
$$\hat{\mathbf{U}}_{cs} = \left[\hat{\mathbf{u}}_1 \ldots \hat{\mathbf{u}}_r\right],\ \hat{\mathbf{U}}_{lns} = \left[\hat{\mathbf{u}}_{r+1} \ldots \hat{\mathbf{u}}_m\right],\ \hat{\mathbf{V}}_{rs} = \left[\hat{\mathbf{v}}_1 \ldots \hat{\mathbf{v}}_r\right],\ \hat{\mathbf{V}}_{ns} = \left[\hat{\mathbf{v}}_{r+1} \ldots \hat{\mathbf{v}}_n\right]$$
- Now, $\mathbf{A}$ can be written as,
$$\mathbf{A} = \begin{bmatrix}\hat{\mathbf{U}}_{cs} & \hat{\mathbf{U}}_{lns}\end{bmatrix} \begin{bmatrix}\mathbf{R} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}\end{bmatrix} \begin{bmatrix}\hat{\mathbf{V}}_{rs}^T \\ \hat{\mathbf{V}}_{ns}^T\end{bmatrix}$$
where, $\mathbf{R} \in \mathbb{R}^{r \times r}$.
It can be shown that two orthogonal matrices $\mathbf{P}$ and $\mathbf{Q}$ can be chosen, such that
$$\mathbf{A} = \begin{bmatrix}\hat{\mathbf{U}}_{cs} & \hat{\mathbf{U}}_{lns}\end{bmatrix} \mathbf{P} \begin{bmatrix}\mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0}\end{bmatrix} \mathbf{Q}^T \begin{bmatrix}\hat{\mathbf{V}}_{rs}^T \\ \hat{\mathbf{V}}_{ns}^T\end{bmatrix} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$$

Singular Value Decomposition: Diagonalizing any matrix

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_m \end{bmatrix} \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \ldots \mathbf{v}_n \end{bmatrix}^T$$

- Orthonormal basis for $C\left(\mathbf{A}\right) \rightarrow \{\mathbf{u}_1 \ldots \mathbf{u}_r\}$.
- Orthonormal basis for $N\left(\mathbf{A}^T\right) \rightarrow \{\mathbf{u}_{r+1} \ldots \mathbf{u}_m\}$.
- Orthonormal basis for $C\left(\mathbf{A}^T\right) \rightarrow \{\mathbf{v}_1 \ldots \mathbf{v}_r\}$.
- Orthonormal basis for $N\left(\mathbf{A}\right) \rightarrow \{\mathbf{v}_{r+1} \ldots \mathbf{v}_n\}$.
- $\mathbf{D} = \begin{bmatrix} \sigma_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \sigma_r \end{bmatrix}, \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0.$
- Reduced SVD: $\mathbf{A} = \begin{bmatrix} \mathbf{u}_1 \ldots \mathbf{u}_r \end{bmatrix} \begin{bmatrix} \sigma_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \sigma_r \end{bmatrix} \begin{bmatrix} \mathbf{v}_1^T \\ \vdots \\ \mathbf{v}_r^T \end{bmatrix}$

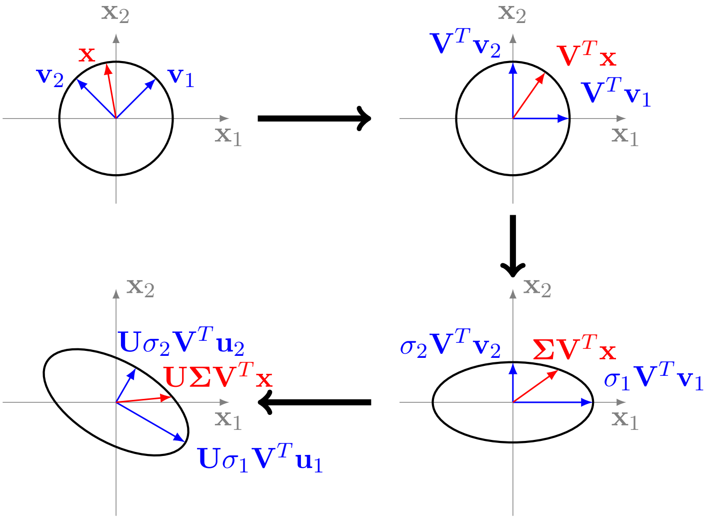
Geometry of SVD

$\mathbf{y} = \mathbf{A}\mathbf{x}$, where $\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$, $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $rank\left(\mathbf{A}\right) = n$.

$$1 = \|\mathbf{x}\|^2 = \left\|\mathbf{A}^{-1}\mathbf{y}\right\|^2$$
$$= \mathbf{y}^T\mathbf{A}^{-T}\mathbf{A}^{-1}\mathbf{y}$$
$$= \mathbf{y}^T\left(\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^T\right)^T\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^T\mathbf{y}$$
$$= \mathbf{y}^T\mathbf{U}\mathbf{\Sigma}^{-1}\mathbf{V}^T\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^T\mathbf{y}$$
$$= \mathbf{w}^T\mathbf{\Sigma}^{-2}\mathbf{w}$$

where, $\mathbf{w} = \mathbf{U}^T\mathbf{y}$;

$$x_1^2 + \ldots + x_n^2 = \frac{w_1^2}{\sigma_1^2} + \frac{w_2^2}{\sigma_2^2} + \ldots + \frac{w_n^2}{\sigma_n^2} = 1$$



Singular Value Decomposition: Diagonalizing any matrix

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \ldots & \mathbf{u}_m \end{bmatrix} \begin{bmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \ldots \mathbf{v}_n \end{bmatrix}^T$$

SVD allows us to obtain low rank approximation of the given matrix $\mathbf{A}$, which has lots of applications in signal processing and data analysis.

$$\mathbf{A} = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \sigma_2 \mathbf{u}_2 \mathbf{v}_2^T + \ldots + \sigma_r \mathbf{u}_r \mathbf{v}_r^T, \;\; rank\,(\mathbf{A}) = r$$

where, $\mathbf{u}_i \mathbf{v}_i^T$ are rank one matrices.
We can obtain a matrix of rank $k < r$ by setting $\sigma_i = 0, \forall k < i \leq r$.

$$\mathbf{A}_k = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \ldots + \sigma_k \mathbf{u}_k \mathbf{v}_k^T$$

SVD gives the best possible low rank approximations in terms of the distance between $\mathbf{A}$ and $\mathbf{A}_k$.

$$\min_{rank(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_2 = \|\mathbf{A} - \mathbf{A}_k\|_2 = \sigma_{k+1}$$

$$\min_{rank(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_F = \|\mathbf{A} - \mathbf{A}_k\|_F = \left(\sum_{i=k+1}^{r} \sigma_i^2 \right)^{1/2}$$

Singular Value Decomposition: Diagonalizing any matrix

- Geometrically, low rank approximations correspond to a r-dimensional hyper-ellipsoid transformed to a lower dimensional hyper-ellipsoid by flattening the r-dimensional hyper-ellipsoid along its smallest principal axis.
- **Principal component analysis**:
    - Multi-dimensional data often have structure in the form of correlations between the individual variables. Such data can be approximated by a lower dimensional representation.