Introduction to SVD

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Outline

Definition

Input: A, a $m \times n$ real matrix.

Output: $A = U\Sigma V^T$ such that

U is a $m \times m$ orthogonal matrix ($UU^T = I_m$)
V is a $n \times n$ orthogonal matrix ($VV^T = I_n$)
Σ is a $m \times n$ diagonal matrix $diag(\sigma_1, \ldots, \sigma_p)$, where $p = min(m, n)$ and $\sigma_1 \geq \ldots \geq \sigma_p \geq 0$.

If A is symmetric and *positive semi-definitive*, then σ_i are eigenvalues of A: there exists $\vec{x}$ s.t. $A\vec{x} = \sigma_i \vec{x}$.

Example

$$A = \begin{bmatrix} 1 & 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \end{bmatrix}$$

$$U = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \Sigma = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$V^T = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ \sqrt{0.2} & 0 & 0 & 0 & \sqrt{0.8} \\ 0 & 0 & 0 & 1 & 0 \\ -\sqrt{0.8} & 0 & 0 & 0 & \sqrt{0.2} \end{bmatrix}$$

Properties

- Any orthogonal matrix is a *rotation*.
- When A is *symmetric*, that is, $A = A^T$, $U = V$
- Find the *minimum-norm least square solution* to a linear system $A\mathbf{x} = \mathbf{b}$

Problem: given $A : m \times n$, $\mathbf{b} : m \times 1$, find the $\mathbf{x} : n \times 1$ that minimizes $\|A\mathbf{x} - \mathbf{b}\|$.

1. Solve the SVD of A, denoted by $A = U\Sigma V^T$.
2. Let $\Sigma^\dagger$ be a $n \times m$ matrix s.t. $\Sigma^\dagger = diag(\frac{1}{\sigma_1}, \ldots, \frac{1}{\sigma_p})$
3. Output $\mathbf{x} = V\Sigma^\dagger U^T \mathbf{b}$.

Example: Line fitting

Problem: let $p_1, \ldots, p_m \in \mathbb{R}^2$, find the line $l : ax + by - 1 = 0$ that minimizes the sum of square distances from p_i to l.

1. The distance from $p_i = (x_i, y_i)$ to l is $d_i = |ax_1 + by_1 - 1|$
2. Let $A = (p_1, \ldots, p_m)^T$, $\mathbf{b} = 1$.
3. Output $\mathbf{x} = (a, b)^T = V\Sigma^\dagger U^T \mathbf{b}$.

For example, 4 points $(0,1), (1,2), (2,4), (3,3)$.

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 2 \\ 2 & 4 \\ 3 & 3 \end{bmatrix}, \mathbf{b} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

SVD and NVR

NVR algorithm has two phases

1. Find an assignment of (≥ 5) peak-residue pairs (initial fixed matchings)
2. (a) For each “candidate" structure in PDB, calculate the Saupe matrix (alignment tensor) S using the fixed matchings(assignments) by SVD
   (b) For each candidate structure, calculate the “back-calculated RDCs"; use it to calculate the weight of unknown edges
   (c) Aggregate the matchings of all candidates’ structure to find the most probable matching(s), add them to the set of fixed matchings
   (d) If not done, go to (a) with the new set of fixed matchings.

Simplified Phase 2

1. Use the fixed matching F to calculate S.
2. Use S to calculate the back-computed RDCs. (SVD is used)
3. Match back-computed RDCs with experimental RDCs. (MBM problem)
4. Aggregate the results of matching of each possible structure (usually < 5), find the most probable edge e.
5. $F \leftarrow F \cup \{e\}$; if F is not a perfect matching, go to 1.

Conclusion

- SVD, $A = U\Sigma T^T$
- Properties: provides a least square solution to a linear system $A\mathbf{x} = \mathbf{b}$
- Used in NVR to compute the alignment tensors of candidate structures to best fit the experimental RDCs, based on fixed assignments (for multiple rounds)