Matrix Decomposition

✓ LU

✓ QR

✓ Spectral (square matrices)

→ SVD

SVD Computation

For all matrices $\underline{A} \in M_{mn}$

$$\underline{A} = \underline{U}\,\underline{\Sigma}\,\underline{V}^T \qquad \underline{A}\,\underline{v} = \sigma\,\underline{u}$$

$\underline{U}$ is $m \times m$ unitary matrix

$\underline{V}$ is $n \times n$ unitary matrix

$\underline{\Sigma}$ is $m \times n$ diagonal matrix with real, non-negative singular values σ_j on the diagonal, ordered such that $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_p \geq 0$ for $p = \min(m, n)$

How can the SVD of $\underline{A}$ be found?

Hand-based calculation for small systems $\rightarrow$ Find eigenvalues and eigenvectors of $\underline{A}^T\underline{A}$ and $\underline{A}\,\underline{A}^T$

① Find all singular values of $\underline{A} \in \mathbb{R}^{m \times n}$

If $m = n$, then use either $\underline{A}^T\underline{A}$ or $\underline{A}\,\underline{A}^T$

If $m < n$, then use $\underline{A}\,\underline{A}^T \in \mathbb{R}^{m \times m}$ since there can be at most m singular values

If $m > n$, then use $\underline{A}^T \underline{A} \in \mathbb{R}^{n \times n}$ since there can be at most n singular values

② Find $\underline{V}$: Eigenvectors of $\underline{A}^T \underline{A}$, append zero eigenvalues as needed

③ Find $\underline{U}$: For those $\sigma_j > 0$, use $\underline{u}_j = \frac{1}{\sigma_j} \underline{A} \underline{v}_j$

For other singular values, determine unitary decomposition of $\underline{A}\underline{A}^T$

Example:

Find SVD of $\underline{A} = \begin{bmatrix} 2 & 1 \\ 1 & -1 \\ 1 & -2 \end{bmatrix}$ $m = 3$, $n = 2$

Determine eigenvalues of $\underline{A}^T \underline{A} = \begin{bmatrix} 6 & -1 \\ -1 & 6 \end{bmatrix}$

$\text{rank}(\underline{A}^T \underline{A}) = 2$

$$\det(\underline{A}^T \underline{A} - \lambda \underline{I}) = (6-\lambda)(6-\lambda) - (-1)^2 = 0$$

$$36 - 12\lambda + \lambda^2 - 1 = 0$$

$$(\lambda - 7)(\lambda - 5) = 0 \rightarrow \lambda_1 = 7 \rightarrow \sigma_1 = \sqrt{7}$$

$$\lambda_2 = 5 \rightarrow \sigma_2 = \sqrt{5}$$

Singular values

$$\lambda_2 = 5 \rightarrow \sigma_2 = \sqrt{5} \Big\} \text{ values}$$

Determine $\underline{V}$

Find eigenvectors of $\underline{A}^T\underline{A}$

$$\lambda_1 = 7, \quad (\underline{A}^T\underline{A} - \lambda_1 \underline{I})\underline{x} = \underline{0}$$

$$\left(\begin{bmatrix} 6 & -1 \\ -1 & 6 \end{bmatrix} - \begin{bmatrix} 7 & 0 \\ 0 & 7 \end{bmatrix} \right) \xrightarrow{\text{rref}} \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \rightarrow \underline{x} = \begin{bmatrix} -1 \\ +1 \end{bmatrix}$$

$$v_1 = \frac{\underline{x}}{\|\underline{x}\|} = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$\lambda_1 = 5, \quad (\underline{A}^T\underline{A} - \lambda_2 \underline{I})\underline{x} = \underline{0}$$

$$\left(\begin{bmatrix} 6 & -1 \\ -1 & 6 \end{bmatrix} - \begin{bmatrix} 5 & 0 \\ 0 & 5 \end{bmatrix} \right) \xrightarrow{\text{rref}} \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix} \rightarrow \underline{x} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$v_2 = \frac{\underline{x}}{\|\underline{x}\|} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

Determine $\underline{U}$

$$\underline{u}_1 = \frac{1}{\sigma_1} \underline{A} v_1 = \frac{1}{\sqrt{7}} \begin{bmatrix} 2 & 1 \\ 1 & -1 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$\underline{u}_1 = \frac{1}{\sqrt{14}} \begin{bmatrix} -2+1 \\ -1-1 \\ -1-2 \end{bmatrix} = \frac{1}{\sqrt{14}} \begin{bmatrix} -1 \\ -2 \\ -3 \end{bmatrix}$$

$$\underline{u}_2 = \frac{1}{\sigma_2} \underline{A}\, \underline{v}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 & 1 \\ 1 & -1 \\ 1 & -2 \end{bmatrix} \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$\underline{u}_2 = \frac{1}{\sqrt{10}} \begin{bmatrix} 2+1 \\ 1-1 \\ 1-2 \end{bmatrix} = \frac{1}{\sqrt{10}} \begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}$$

$$\underline{u}_3 : \quad \underline{A}\underline{A}^T = \begin{bmatrix} 5 & 1 & 0 \\ 1 & 2 & 3 \\ 0 & 3 & 5 \end{bmatrix} \xrightarrow{\text{rref}} \begin{bmatrix} 1 & 0 & -1/3 \\ 0 & 1 & 5/3 \\ 0 & 0 & 0 \end{bmatrix}$$

Let $x_3 = 1 \rightarrow x_1 = \frac{1}{3}, \ x_2 = -\frac{5}{3}$

$$\underline{u}_3 = \frac{\underline{x}}{\|\underline{x}\|} \Rightarrow \underline{x} = \frac{1}{3} \begin{bmatrix} 1 \\ -5 \\ 3 \end{bmatrix}, \ \|\underline{x}\| = \frac{1}{3}\left(1+25+9\right)^{1/2}$$

$$\underline{u}_3 = \frac{3}{\sqrt{35}} \begin{bmatrix} 1/3 \\ -5/3 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{35}} \begin{bmatrix} 1 \\ -5 \\ 3 \end{bmatrix}$$

SVD of $\underset{3\times 2}{\underline{A}} = \underset{3\times 3}{\underline{U}}\ \underset{3\times 2}{\underline{\Sigma}}\ \underset{2\times 2}{\underline{V}}^T$

$$\underline{U} = \begin{bmatrix} -1/\sqrt{14} & 3/\sqrt{10} & 1/\sqrt{35} \\ -2/\sqrt{14} & 0 & -5/\sqrt{35} \\ -3/\sqrt{14} & -1/\sqrt{10} & 3/\sqrt{35} \end{bmatrix}, \quad \underline{V} = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$$\underline{\Sigma} = \begin{bmatrix} \sqrt{7} & 0 \\ 0 & \sqrt{5} \\ 0 & 0 \end{bmatrix}$$

Matlab: $[U, S, V] = \text{svd}(A)$

```
U =

  -0.267261241912424   0.948683298050514   0.169030850945703
  -0.534522483824849   0.000000000000000  -0.845154254728516
  -0.801783725737273  -0.316227766016837   0.507092552837110


S =

   2.645751311064591                   0
                   0   2.236067977499789
                   0                   0


V =

  -0.707106781186547   0.707106781186548
   0.707106781186548   0.707106781186547
```

Computing SVD for General $\underline{A}$

Let $\underline{A} \in \mathbb{R}^{m \times n}$

Naive Method:

① Compute eigendecomposition of $\underline{A}^T\underline{A}$

$$\underline{A}^T\underline{A} = \underline{V}\,\underline{\Lambda}\,\underline{V}^T$$

② $\underline{\Sigma} = \underline{\Lambda}^{1/2}$ for $m = n$

In general, $\sigma_j = (\lambda_j)^{1/2}$, with $\underline{\Sigma} = \text{diag}(\underline{\sigma})$

③ Solve $\underline{U}\,\underline{\Sigma} = \underline{A}\,\underline{V}$ for $\underline{U}$

$\Rightarrow$ Condition number of $\underline{A}^T\underline{A}$ is large

$\Rightarrow$ Loss of accuracy, if $\sigma_k \ll \|\underline{A}\|$

Instead, use iterative methods

Two-step process

① Convert $\underline{A}$ to bi-diagonal form

② Convert bi-diagonal to diagonal

$$\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \xrightarrow{①} \begin{bmatrix} \times & \times & 0 \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix} \xrightarrow{②} \begin{bmatrix} \times & 0 & 0 \\ 0 & \times & 0 \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix}$$

Golub-Kahan (G-K) Bidiagonalization

Use Householder on both left and right

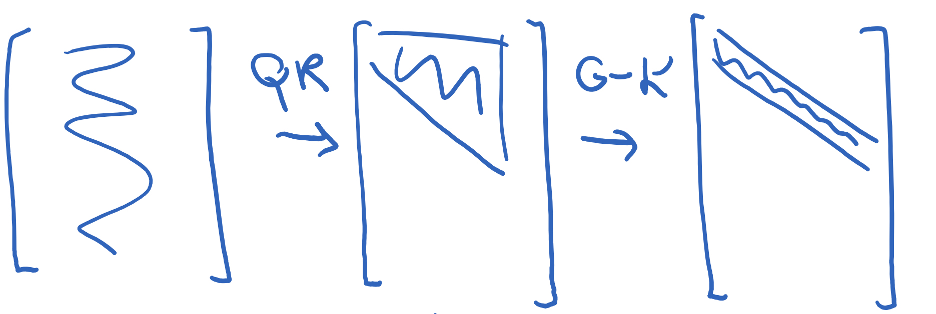
$$\underset{\underline{A}\ (m \times n)}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}} \xrightarrow{\underline{U}_1^T} \underset{\underline{U}_1^T \underline{A}}{\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}} \xrightarrow{\underline{V}_1} \underset{\underline{U}_1^T \underline{A}\,\underline{V}_1}{\begin{bmatrix} \times & \times & 0 \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}}$$

Operation count $\sim 4mn^2 - \frac{4}{3}n^3$

$\sim 2\times$ that of QR decomposition, but result is close to final $\underline{R}$

Alternative: Lawson-Hanson-Chan (LHC)

Do QR on $\underline{A}$ first, then G-K on the $\underline{R}$ matrix



$\underline{A}$ $\qquad$ $\underline{Q}^T\underline{A}$ $\qquad$ $\underline{U}^T\underline{Q}^T\underline{A}\,\underline{V}$

Operation count for LHC

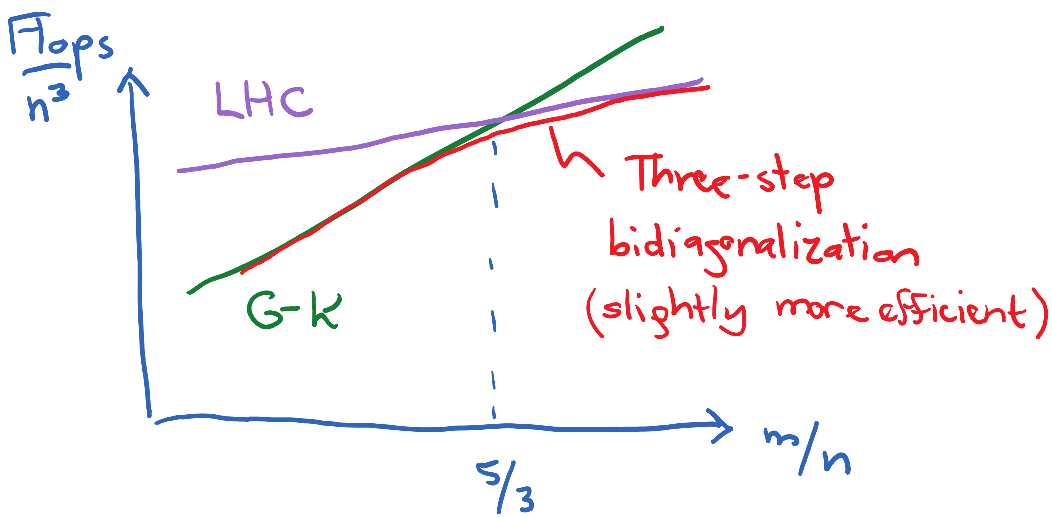
$$QR \sim 2mn^2 - \frac{2}{3}n^3$$

$$G\text{-}K \sim \frac{8}{3}n^3$$

$$\text{Total} \sim 2mn^2 + 2n^3$$

$\therefore$ LHC is cheaper than straight G-K,

if $m > \frac{5}{3}n$



See Trefethen + Bau, Lecture 31

for more detail

$\underline{A}\,\underline{x} = \underline{b}$ might arise from linear systems of equations, regression, etc.

Consider $\underline{A} \in \mathbb{R}^{m \times n}$

① LU Decomposition $\underline{A} = \underline{L}\,\underline{U}$

$\underline{L}$: lower triangular

$\underline{U}$: upper triangular

To decompose $\underline{A} = \underline{L}\,\underline{U}$ used Gaussian elimination

$\underline{A}\,\underline{x} = \underline{b}$

$\underline{L}\,\underline{U}\,\underline{x} = \underline{b}$ Obtain LU decomposition

$\underline{U}\,\underline{x} = \underline{L}^{-1}\underline{b}$ Forward substitution

$\underline{x} = \underline{U}^{-1}(\underline{L}^{-1}\underline{b})$ Backward substitution

② QR Decomposition $\underline{A} = \underline{Q}\,\underline{R}$

$$\underline{Q}^T \underline{Q} = \underline{I}$$

$\underline{R}$: upper triangular

To decompose $\underline{A} = \underline{Q}\,\underline{R}$

Classical Gram-Schmidt

Modified Gram-Schmidt

Householder

More stable, more expensive

$$\underline{A}\,\underline{x} = \underline{b}$$

$$\underline{Q}\,\underline{R}\,x = \underline{b} \qquad \text{Obtain QR decomposition}$$

$$\underline{R}\,\underline{x} = \underline{Q}^T \underline{b} \qquad \text{Orthogonalize}$$

$$\underline{x} = \underline{R}^{-1} \underline{Q}^T \underline{b} \qquad \text{Forward substitution}$$

③ Spectral Decomposition (Eigensystems)

All square matrices: $\underline{A} = \underline{Q}\,\underline{T}\,\underline{Q}^T$

$\underline{T}$: Upper triangular with eigenvalues on diagonal

diagonal

$\underset{\sim}{Q}$: Unitary $(\underset{\sim}{Q}^T \underset{\sim}{Q} = \underset{\sim}{Q}\underset{\sim}{Q}^T = \underset{\sim}{I})$

Schur Decomposition

$$\underset{\sim}{A} = \underset{\sim}{Q}\underset{\sim}{T}\underset{\sim}{Q}^T$$

$$\underset{\sim}{Q}^T \underset{\sim}{A}\underset{\sim}{Q} = \underset{\sim}{Q}^T\underset{\sim}{Q}\underset{\sim}{T}\underset{\sim}{Q}^T\underset{\sim}{Q}$$

$$\underset{\sim}{Q}^T \underset{\sim}{A}\underset{\sim}{Q} = \underset{\sim}{T}$$

If $\underset{\sim}{A}$ is complete: $\underset{\sim}{A} = \underset{\sim}{S}\underset{\sim}{\Lambda}\underset{\sim}{S}^{-1}$

$\underset{\sim}{\Lambda}$: Diagonal matrix with eigenvalues on diagonal

$\underset{\sim}{S}$: Eigenvectors in columns

If $\underset{\sim}{A}$ is normal: $\underset{\sim}{A} = \underset{\sim}{Q}\underset{\sim}{\Lambda}\underset{\sim}{Q}^T$

$\underset{\sim}{\Lambda}$: Diagonal matrix with eigenvalues on diagonal

$\underset{\sim}{Q}$: Unitary $(\underset{\sim}{Q}^T \underset{\sim}{Q} = \underset{\sim}{Q}\underset{\sim}{Q}^T = \underset{\sim}{I})$

Diagonalization of $\underline{A}$

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

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

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

$$\therefore \underline{Q}^T\underline{A}\,\underline{Q} = \underline{\Lambda} \quad \text{(diagonal)}$$

④ Singular Value Decomposition

$$\underline{A} = \underline{U}\,\underline{\Sigma}\,\underline{V}^T \qquad \underline{U}^T\underline{U} = \underline{U}\,\underline{U}^T = \underline{I}$$

$$\underline{V}^T\underline{V} = \underline{V}\,\underline{V}^T = \underline{I}$$

$\underline{\Sigma}$: diagonal matrix

Methods: Golub-Kahan (-Lanczos)

Lawson-Hanson-Chan

$$\underline{A}\,\underline{x} = \underline{b}$$

$$\underline{U}\,\underline{\Sigma}\,\underline{V}^T\underline{x} = \underline{b} \qquad \text{Obtain SVD}$$

$$\underline{\Sigma}\,\underline{V}^T\underline{x} = \underline{U}^T\underline{b}$$ Unitary $\underline{U}$

$$\underline{V}^T\underline{x} = \underline{\Sigma}^{-1}\underline{U}^T\underline{b}$$ Diagonal $\underline{\Sigma}$

$$\underline{x} = \underbrace{\underline{V}\,\underline{\Sigma}^{-1}\underline{U}^T}_{\text{Pseudo-inverse of } \underline{A}}\underline{b}$$ Unitary $\underline{V}$

Methods

Increasing stability + Increasing cost ↓

LU – Gaussian elim.

QR – Classical G-S

QR – Modified G-S

QR – Householder

SVD – G-K/LHC

Note: Some automatically solve the normal equations

$$\underline{A}^T\underline{A}\,\underline{x} = \underline{A}^T\underline{b}$$