ENGG5781 Matrix Analysis and Computations
Lecture 5: Singular Value Decomposition

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Lecture 5: Singular Value Decomposition

- singular value decomposition
- matrix norms
- linear systems
- LS, pseudo-inverse, orthogonal projections
- low-rank matrix approximation
- singular value inequalities
- computing the SVD via the power method

Main Results

- any matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ admits a singular value decomposition

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

where $\mathbf{U} \in \mathbb{R}^{m \times m}$ and $\mathbf{V} \in \mathbb{R}^{m \times m}$ are orthogonal, and $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$ has $[\mathbf{\Sigma}]_{ij} = 0$ for all $i \neq j$ and $[\mathbf{\Sigma}]_{ii} = \sigma_i$ for all i, with $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_{\min\{m,n\}}$.

- matrix 2-norm: $\|\mathbf{A}\|_2 = \sigma_1$

- let r be the number of nonzero σ_i's, partition $\mathbf{U} = [\ \mathbf{U}_1\ \mathbf{U}_2\ ]$, $\mathbf{V} = [\ \mathbf{V}_1\ \mathbf{V}_2\ ]$, and let $\tilde{\mathbf{\Sigma}} = \mathrm{Diag}(\sigma_1, \ldots, \sigma_r)$
  - pseudo-inverse: $\mathbf{A}^\dagger = \mathbf{V}_1 \tilde{\mathbf{\Sigma}}^{-1} \mathbf{U}_1^T$
  - LS solution: $\mathbf{x}_{\sf LS} = \mathbf{A}^\dagger \mathbf{y} + \boldsymbol{\eta}$ for any $\boldsymbol{\eta} \in \mathcal{R}(\mathbf{V}_2)$
  - orthogonal projection: $\mathbf{P}_{\mathbf{A}} = \mathbf{U}_1 \mathbf{U}_1^T$

Main Results

- low-rank matrix approximation: given $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $k \in \{1, \ldots, \min\{m, n\}\}$, the problem

$$\min_{\mathbf{B} \in \mathbb{R}^{m \times n},\ \mathrm{rank}(\mathbf{B}) \leq k} \quad \|\mathbf{A} - \mathbf{B}\|_F^2$$

has a solution given by $\mathbf{B}^\star = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$

Singular Value Decomposition

Theorem 5.1. Given any $\mathbf{A} \in \mathbb{R}^{m \times n}$, there exists a 3-tuple $(\mathbf{U}, \mathbf{\Sigma}, \mathbf{V}) \in \mathbb{R}^{m \times m} \times \mathbb{R}^{m \times n} \times \mathbb{R}^{n \times n}$ such that

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

$\mathbf{U}$ and $\mathbf{V}$ are orthogonal, and $\mathbf{\Sigma}$ takes the form

$$[\mathbf{\Sigma}]_{ij} = \begin{cases} \sigma_i, & i = j \\ 0, & i \neq j \end{cases}, \qquad \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_p \geq 0, \;\; p = \min\{m, n\}.$$

- the above decomposition is called the singular value decomposition (SVD)
- σ_i is called the ith singular value
- $\mathbf{u}_i$ and $\mathbf{v}_i$ are called the ith left and right singular vectors, resp.
- the following notations may be used to denote singular values of a given $\mathbf{A}$

$$\sigma_{\max}(\mathbf{A}) = \sigma_1(\mathbf{A}) \geq \sigma_2(\mathbf{A}) \geq \ldots \geq \sigma_p(\mathbf{A}) = \sigma_{\min}(\mathbf{A})$$

Different Ways of Writing out SVD

- partitioned form: let r be the number of nonzero singular values, and note $\sigma_1 \geq \ldots \sigma_r > 0$, $\sigma_{r+1} = \ldots = \sigma_p = 0$. Then,

$$\mathbf{A} = \begin{bmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{\Sigma}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{V}_1^T \\ \mathbf{V}_2^T \end{bmatrix},$$

  where

  - $\tilde{\mathbf{\Sigma}} = \mathrm{Diag}(\sigma_1, \ldots, \sigma_r)$,
  - $\mathbf{U}_1 = [\ \mathbf{u}_1, \ldots, \mathbf{u}_r\ ] \in \mathbb{R}^{m \times r}$, $\mathbf{U}_2 = [\ \mathbf{u}_{r+1}, \ldots, \mathbf{u}_m\ ] \in \mathbb{R}^{m \times (m-r)}$,
  - $\mathbf{V}_1 = [\ \mathbf{v}_1, \ldots, \mathbf{v}_r\ ] \in \mathbb{R}^{n \times r}$, $\mathbf{V}_2 = [\ \mathbf{v}_{r+1}, \ldots, \mathbf{v}_n\ ] \in \mathbb{R}^{n \times (n-r)}$.

- thin SVD: $\mathbf{A} = \mathbf{U}_1 \tilde{\mathbf{\Sigma}} \mathbf{V}_1^T$

- outer-product form: $\mathbf{A} = \sum_{i=1}^{p} \sigma_i \mathbf{u}_i \mathbf{v}_i^T = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$

SVD and Eigendecomposition

From the SVD $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$, we see that

$$\mathbf{A}\mathbf{A}^T = \mathbf{U}\mathbf{D}_1\mathbf{U}^T, \qquad \mathbf{D}_1 = \boldsymbol{\Sigma}\boldsymbol{\Sigma}^T = \mathrm{Diag}(\sigma_1^2, \ldots, \sigma_p^2, \underbrace{0, \ldots, 0}_{m-p \text{ zeros}}) \qquad (*)$$

$$\mathbf{A}^T\mathbf{A} = \mathbf{V}\mathbf{D}_2\mathbf{V}^T, \qquad \mathbf{D}_2 = \boldsymbol{\Sigma}^T\boldsymbol{\Sigma} = \mathrm{Diag}(\sigma_1^2, \ldots, \sigma_p^2, \underbrace{0, \ldots, 0}_{n-p \text{ zeros}}) \qquad (**)$$

Observations:

- $(*)$ and $(**)$ are the eigendecompositions of $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$, resp.
- the left singular matrix $\mathbf{U}$ of $\mathbf{A}$ is the eigenvector matrix of $\mathbf{A}\mathbf{A}^T$
- the right singular matrix $\mathbf{V}$ of $\mathbf{A}$ is the eigenvector matrix of $\mathbf{A}^T\mathbf{A}$
- the squares of nonzero singular values of $\mathbf{A}$, $\sigma_1^2, \ldots, \sigma_r^2$, are the nonzero eigenvalues of both $\mathbf{A}\mathbf{A}^T$ and $\mathbf{A}^T\mathbf{A}$.

Insights of the Proof of SVD

- the proof of SVD is constructive
- to see the insights, consider the special case of square nonsingular $\mathbf{A}$
- $\mathbf{A}\mathbf{A}^T$ is PD, and denote its eigendecomposition by

$$\mathbf{A}\mathbf{A}^T = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^T, \qquad \text{with } \lambda_1 \geq \ldots \geq \lambda_n > 0.$$

- let $\boldsymbol{\Sigma} = \mathrm{Diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_m})$, $\mathbf{V} = \mathbf{A}^T\mathbf{U}\boldsymbol{\Sigma}^{-1}$
- it can be verified that $\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{A}$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}$
- see the accompanying note for the proof of SVD in the general case

SVD and Subspace

Property 5.1. The following properties hold:

(a) $\mathcal{R}(\mathbf{A}) = \mathcal{R}(\mathbf{U}_1)$, $\mathcal{R}(\mathbf{A})^\perp = \mathcal{R}(\mathbf{U}_2)$;

(b) $\mathcal{R}(\mathbf{A}^T) = \mathcal{R}(\mathbf{V}_1)$, $\mathcal{R}(\mathbf{A}^T)^\perp = \mathcal{N}(\mathbf{A}) = \mathcal{R}(\mathbf{V}_2)$;

(c) $\mathrm{rank}(\mathbf{A}) = r$ (the number of nonzero singular values).

Note:

- in practice, SVD can be used a numerical tool for computing bases of $\mathcal{R}(\mathbf{A})$, $\mathcal{R}(\mathbf{A})^\perp$, $\mathcal{R}(\mathbf{A}^T)$, $\mathcal{N}(\mathbf{A})$
- we have previously learnt the following properties
  - $\mathrm{rank}(\mathbf{A}^T) = \mathrm{rank}(\mathbf{A})$
  - $\dim \mathcal{N}(\mathbf{A}) = n - \mathrm{rank}(\mathbf{A})$

  By SVD, the above properties are easily seen to be true

Matrix Norms

- the definition of a norm of a matrix is the same as that of a vector:
  - $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ is a norm if (i) $f(\mathbf{A}) \geq 0$ for all $\mathbf{A}$; (ii) $f(\mathbf{A}) = 0$ if and only if $\mathbf{A} = \mathbf{0}$; (iii) $f(\mathbf{A}+\mathbf{B}) \leq f(\mathbf{A}) + f(\mathbf{B})$ for any $\mathbf{A}, \mathbf{B}$; (iv) $f(\alpha\mathbf{A}) = |\alpha| f(\mathbf{A})$ for any $\alpha, \mathbf{A}$
- naturally, the Frobenius norm $\|\mathbf{A}\|_F = \sqrt{\sum_{i,j} |a_{ij}|^2} = [\mathrm{tr}(\mathbf{A}^T\mathbf{A})]^{1/2}$ is a norm
- there are many other matrix norms
- induced norm or operator norm: the function

$$f(\mathbf{A}) = \max_{\|\mathbf{x}\|_\beta \leq 1} \|\mathbf{A}\mathbf{x}\|_\alpha$$

where $\|\cdot\|_\alpha, \|\cdot\|_\beta$ denote any vector norms, can be shown be to a norm

Matrix Norms

- matrix norms induced by the vector p-norm ($p \geq 1$):

$$\|\mathbf{A}\|_p = \max_{\|\mathbf{x}\|_p \leq 1} \|\mathbf{A}\mathbf{x}\|_p$$

- it is known that
  - $\|\mathbf{A}\|_1 = \max_{1 \leq j \leq n} \sum_{i=1}^m |a_{ij}|$
  - $\|\mathbf{A}\|_\infty = \max_{1 \leq i \leq m} \sum_{j=1}^n |a_{ij}|$

- how about $p = 2$?

Matrix 2-Norm

- matrix 2-norm or spectral norm:

$$\|\mathbf{A}\|_2 = \sigma_{\max}(\mathbf{A}).$$

- proof:
  - for any $\mathbf{x}$ with $\|\mathbf{x}\|_2 \le 1$,

$$\begin{aligned} \|\mathbf{A}\mathbf{x}\|_2^2 &= \|\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{x}\|_2^2 = \|\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{x}\|_2^2 \\ &\le \sigma_1^2\|\mathbf{V}^T\mathbf{x}\|_2^2 = \sigma_1^2\|\mathbf{x}\|_2^2 \le \sigma_1^2 \end{aligned}$$

  - $\|\mathbf{A}\mathbf{x}\|_2 = \sigma_1$ if we choose $\mathbf{x} = \mathbf{v}_1$

- implication to linear systems: let $\mathbf{y} = \mathbf{A}\mathbf{x}$ be a linear system. Under the input energy constraint $\|\mathbf{x}\|_2 \le 1$, the system output energy $\|\mathbf{y}\|_2^2$ is maximized when $\mathbf{x}$ is chosen as the 1st right singular vector

- corollary: $\min_{\|\mathbf{x}\|_2 = 1} \|\mathbf{A}\mathbf{x}\|_2 = \sigma_{\min}(\mathbf{A})$ if $m \ge n$

Matrix 2-Norm

Properties for the matrix 2-norm:

- $\|\mathbf{AB}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{B}\|_2$
  - in fact, $\|\mathbf{AB}\|_p \leq \|\mathbf{A}\|_p \|\mathbf{B}\|_p$ for any $p \geq 1$
- $\|\mathbf{Ax}\|_2 \leq \|\mathbf{A}\|_2 \|\mathbf{x}\|_2$
  - a special case of the 1st property
- $\|\mathbf{QAW}\|_2 = \|\mathbf{A}\|_2$ for any orthogonal $\mathbf{Q}, \mathbf{W}$
  - we also have $\|\mathbf{QAW}\|_F = \|\mathbf{A}\|_F$ for any orthogonal $\mathbf{Q}, \mathbf{W}$
- $\|\mathbf{A}\|_2 \leq \|\mathbf{A}\|_F \leq \sqrt{p}\|\mathbf{A}\|_2$ (here $p = \min\{m, n\}$)
  - proof: $\|\mathbf{A}\|_F = \|\mathbf{\Sigma}\|_F = \sqrt{\sum_{i=1}^p \sigma_i^2}$, and $\sigma_1^2 \leq \sum_{i=1}^p \sigma_i^2 \leq p\sigma_1^2$

Schatten p-Norm

- the function

$$f(\mathbf{A}) = \left(\sum_{i=1}^{\min\{m,n\}} \sigma_i(\mathbf{A})^p \right)^{1/p}, \qquad p \geq 1,$$

is known to be a norm and is called the Schatten p-norm (how to prove it?).

- nuclear norm:

$$\|\mathbf{A}\|_* = \sum_{i=1}^{\min\{m,n\}} \sigma_i(\mathbf{A})$$

  - a special case of the Schatten p-norm
  - a way to prove that the nuclear norm is a norm:
    - show that $f(\mathbf{A}) = \max_{\|\mathbf{B}\|_2 \leq 1} \mathrm{tr}(\mathbf{B}^T \mathbf{A})$ is a norm
    - show that $f(\mathbf{A}) = \sum_{i=1}^{\min\{m,n\}} \sigma_i$
  - finds applications in rank approximation, e.g., for compressive sensing and matrix completion **[Recht-Fazel-Parrilo'10]**

Schatten p-Norm

- $\text{rank}(\mathbf{A})$ is nonconvex in $\mathbf{A}$ and is arguably hard to do optimization with it
- Idea: the rank function can be expressed as

$$\text{rank}(\mathbf{A}) = \sum_{i=1}^{\min\{m,n\}} \mathbb{1}\{\sigma_i(\mathbf{A}) \neq 0\},$$

  and why not approximate it by

$$f(\mathbf{A}) = \textstyle\sum_{i=1}^{\min\{m,n\}} \varphi(\sigma_i(\mathbf{A}))$$

  for some friendly function φ?

- nuclear norm

$$\|\mathbf{A}\|_* = \textstyle\sum_{i=1}^{\min\{m,n\}} \sigma_i(\mathbf{A})$$

  – uses $\varphi(z) = z$

  – is convex in $\mathbf{A}$

Linear Systems: Sensitivity Analysis

- Scenario:
  - let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be nonsingular, and $\mathbf{y} \in \mathbb{R}^n$. Let $\mathbf{x}$ be the solution to

$$\mathbf{y} = \mathbf{A}\mathbf{x}.$$

  - consider a perturbed version of the above system: $\hat{\mathbf{A}} = \mathbf{A} + \Delta\mathbf{A}, \hat{\mathbf{y}} = \mathbf{y} + \Delta\mathbf{y}$, where $\Delta\mathbf{A}$ and $\Delta\mathbf{y}$ are errors. Let $\hat{\mathbf{x}}$ be a solution to the perturbed system

$$\hat{\mathbf{y}} = \hat{\mathbf{A}}\hat{\mathbf{x}}.$$

- Problem: analyze how the solution error $\|\hat{\mathbf{x}} - \mathbf{x}\|_2$ scales with $\Delta\mathbf{A}$ and $\Delta\mathbf{y}$

- remark: $\Delta\mathbf{A}$ and $\Delta\mathbf{y}$ may be floating point errors, measurement errors, etc

Linear Systems: Sensitivity Analysis

- the condition number of a given matrix $\mathbf{A}$ is defined as

$$\kappa(\mathbf{A}) = \frac{\sigma_{\max}(\mathbf{A})}{\sigma_{\min}(\mathbf{A})},$$

- $\kappa(\mathbf{A}) \geq 1$, and $\kappa(\mathbf{A}) = 1$ if $\mathbf{A}$ is orthogonal

- $\mathbf{A}$ is said to be ill-conditioned if $\kappa(\mathbf{A})$ is very large; that refers to cases where $\mathbf{A}$ is close to singular

Linear Systems: Sensitivity Analysis

Theorem 5.2. Let $\varepsilon > 0$ be a constant such that

$$\frac{\|\Delta \mathbf{A}\|_2}{\|\mathbf{A}\|_2} \leq \varepsilon, \qquad \frac{\|\Delta \mathbf{y}\|_2}{\|\mathbf{y}\|_2} \leq \varepsilon.$$

If ε is sufficiently small such that $\varepsilon\kappa(\mathbf{A}) < 1$, then

$$\frac{\|\hat{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2} \leq \frac{2\varepsilon\kappa(\mathbf{A})}{1 - \varepsilon\kappa(\mathbf{A})}.$$

- Implications:
  - for small errors and in the worst-case sense, the relative error $\|\hat{\mathbf{x}} - \mathbf{x}\|_2 / \|\mathbf{x}\|_2$ tends to increase with the condition number
  - in particular, for $\varepsilon\kappa(\mathbf{A}) \leq \frac{1}{2}$, the error bound can be simplified to

$$\frac{\|\hat{\mathbf{x}} - \mathbf{x}\|_2}{\|\mathbf{x}\|_2} \leq 4\varepsilon\kappa(\mathbf{A})$$

Linear Systems: Interpretation under SVD

- consider the linear system

$$\mathbf{y} = \mathbf{A}\mathbf{x}$$

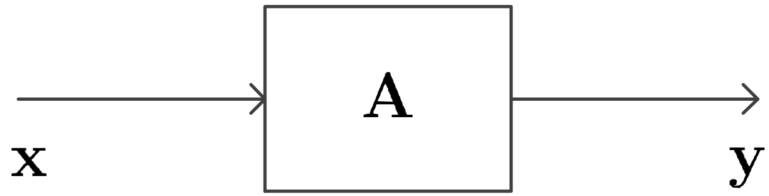
  where $\mathbf{A} \in \mathbb{R}^{m \times n}$ is the system matrix; $\mathbf{x} \in \mathbb{R}^n$ is the system input; $\mathbf{y} \in \mathbb{R}^m$ is the system output

- by SVD we can write

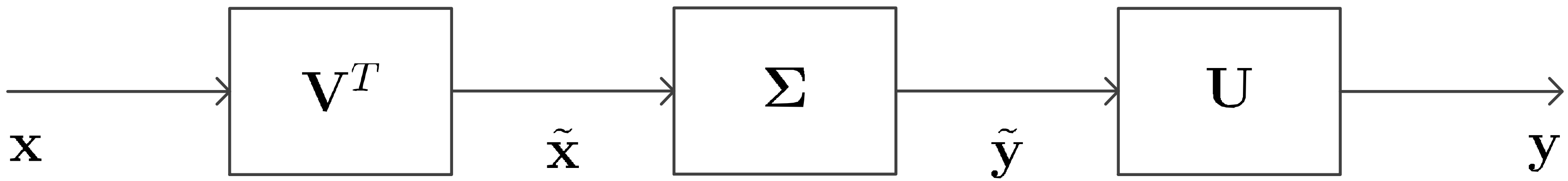
$$\mathbf{y} = \mathbf{U}\tilde{\mathbf{y}}, \qquad \tilde{\mathbf{y}} = \boldsymbol{\Sigma}\tilde{\mathbf{x}}, \qquad \tilde{\mathbf{x}} = \mathbf{V}^T\mathbf{x}$$

- **Implication:** *all* linear systems work by performing three processes in cascade, namely,
  - rotate/reflect the system input $\mathbf{x}$ to form an intermediate system input $\tilde{\mathbf{x}}$
  - form an intermediate system output $\tilde{\mathbf{y}}$ by element-wise rescaling $\tilde{\mathbf{x}}$ w.r.t. σ_i's and by either removing some entires of $\tilde{\mathbf{x}}$ or adding some zeros
  - rotate/reflect $\tilde{\mathbf{y}}$ to form the system output $\mathbf{y}$

Linear Systems: Interpretation under SVD



(a) linear system



(b) equivalent system

Linear Systems: Solution via SVD

- Problem: given *general* $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $\mathbf{y} \in \mathbb{R}^m$, determine
  - whether $\mathbf{y} = \mathbf{A}\mathbf{x}$ has a solution (more precisely, whether there exists an $\mathbf{x}$ such that $\mathbf{y} = \mathbf{A}\mathbf{x}$);
  - what is the solution

- by SVD it can be shown that

$$
\begin{aligned}
\mathbf{y} = \mathbf{A}\mathbf{x} \quad & \Longleftrightarrow \quad \mathbf{y} = \mathbf{U}_1 \tilde{\boldsymbol{\Sigma}} \mathbf{V}_1^T \mathbf{x} \\
& \Longleftrightarrow \quad \mathbf{U}_1^T \mathbf{y} = \tilde{\boldsymbol{\Sigma}} \mathbf{V}_1^T \mathbf{x}, \ \mathbf{U}_2^T \mathbf{y} = \mathbf{0} \\
& \Longleftrightarrow \quad \mathbf{V}_1^T \mathbf{x} = \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}_1^T \mathbf{y}, \ \mathbf{U}_2^T \mathbf{y} = \mathbf{0} \\
& \Longleftrightarrow \quad \begin{array}{l} \mathbf{x} = \mathbf{V}_1 \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}_1^T \mathbf{y} + \boldsymbol{\eta}, \ \text{for any } \boldsymbol{\eta} \in \mathcal{R}(\mathbf{V}_2) = \mathcal{N}(\mathbf{A}), \\ \mathbf{U}_2^T \mathbf{y} = \mathbf{0} \end{array}
\end{aligned}
$$

Linear Systems: Solution via SVD

- let us consider specific cases of the linear system solution characterization

$$\mathbf{y} = \mathbf{A}\mathbf{x} \quad \Longleftrightarrow \quad \begin{array}{l} \mathbf{x} = \mathbf{V}_1 \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}_1^T \mathbf{y} + \boldsymbol{\eta}, \text{ for any } \boldsymbol{\eta} \in \mathcal{R}(\mathbf{V}_2) = \mathcal{N}(\mathbf{A}), \\ \mathbf{U}_2^T \mathbf{y} = \mathbf{0} \end{array}$$

- Case (a): full-column rank $\mathbf{A}$, i.e., $r = n \leq m$
  - there is no $\mathbf{V}_2$, and $\mathbf{U}_2^T \mathbf{y} = \mathbf{0}$ is equivalent to $\mathbf{y} \in \mathcal{R}(\mathbf{U}_1) = \mathcal{R}(\mathbf{A})$
  - Result: the linear system has a solution if and only if $\mathbf{y} \in \mathcal{R}(\mathbf{A})$, and the solution, if exists, is uniquely given by $\mathbf{x} = \mathbf{V} \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}_1^T \mathbf{y}$

- Case (b): full-row rank $\mathbf{A}$, i.e., $r = m \leq n$
  - there is no $\mathbf{U}_2$
  - Result: the linear system always has a solution, and the solution is given by $\mathbf{x} = \mathbf{V}_1 \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}^T \mathbf{y} + \boldsymbol{\eta}$ for any $\boldsymbol{\eta} \in \mathcal{N}(\mathbf{A})$

Least Squares via SVD

- consider the LS problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2$$

for *general* $\mathbf{A}\in\mathbb{R}^{m\times n}$

- we have, for any $\mathbf{x}\in\mathbb{R}^n$,

$$\begin{aligned}\|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2 &= \|\mathbf{y}-\mathbf{U}\boldsymbol{\Sigma}\underbrace{\mathbf{V}^T\mathbf{x}}_{=\tilde{\mathbf{x}}}\|_2^2 = \|\underbrace{\mathbf{U}^T\mathbf{y}}_{=\tilde{\mathbf{y}}}-\boldsymbol{\Sigma}\tilde{\mathbf{x}}\|_2^2 \\ &= \textstyle\sum_{i=1}^r |\tilde{y}_i-\sigma_i\tilde{x}_i|^2 + \sum_{i=r+1}^p |\tilde{y}_i|^2 \\ &\geq \textstyle\sum_{i=r+1}^p |\tilde{y}_i|^2\end{aligned}$$

- the equality above is attained if $\tilde{\mathbf{x}}$ satisfies $\tilde{y}_i=\sigma_i\tilde{x}_i$ for $i=1,\ldots,r$, and it can be shown that such a $\tilde{\mathbf{x}}$ corresponds to (try)

$$\mathbf{x}=\mathbf{V}_1\tilde{\boldsymbol{\Sigma}}^{-1}\mathbf{U}_1^T\mathbf{y}+\mathbf{V}_2\tilde{\mathbf{x}}_2, \quad \text{for any } \tilde{\mathbf{x}}_2\in\mathbb{R}^{n-r}$$

which is the desired LS solution

Pseudo-Inverse

The pseudo-inverse of a matrix $\mathbf{A}$ is defined as

$$\mathbf{A}^\dagger = \mathbf{V}_1 \tilde{\boldsymbol{\Sigma}}^{-1} \mathbf{U}_1^T.$$

From the above def. we can show that

- $\mathbf{x}_{\sf LS} = \mathbf{A}^\dagger \mathbf{y} + \boldsymbol{\eta}$ for any $\boldsymbol{\eta} \in \mathcal{R}(\mathbf{V}_2)$; the same applies to linear sys. $\mathbf{y} = \mathbf{A}\mathbf{x}$
- $\mathbf{A}^\dagger$ satisfies the Moore-Penrose conditions: (i) $\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}$; (ii) $\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger$; (iii) $\mathbf{A}\mathbf{A}^\dagger$ is symmetric; (iv) $\mathbf{A}^\dagger\mathbf{A}$ is symmetric
- when $\mathbf{A}$ has full column rank
  - the pseudo-inverse also equals $\mathbf{A}^\dagger = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$
  - $\mathbf{A}^\dagger\mathbf{A} = \mathbf{I}$
- when $\mathbf{A}$ has full row rank
  - the pseudo-inverse also equals $\mathbf{A}^\dagger = \mathbf{A}^T(\mathbf{A}\mathbf{A}^T)^{-1}$
  - $\mathbf{A}\mathbf{A}^\dagger = \mathbf{I}$

Orthogonal Projections

- with SVD, the orthogonal projections of $\mathbf{y}$ onto $\mathcal{R}(\mathbf{A})$ and $\mathcal{R}(\mathbf{A})^\perp$ are, resp.,

$$\Pi_{\mathcal{R}(\mathbf{A})}(\mathbf{y}) = \mathbf{A}\mathbf{x}_{\sf LS} = \mathbf{A}\mathbf{A}^\dagger\mathbf{y} = \mathbf{U}_1\mathbf{U}_1^T\mathbf{y}$$

$$\Pi_{\mathcal{R}(\mathbf{A})^\perp}(\mathbf{y}) = \mathbf{y} - \mathbf{A}\mathbf{x}_{\sf LS} = (\mathbf{I} - \mathbf{A}\mathbf{A}^\dagger)\mathbf{y} = \mathbf{U}_2\mathbf{U}_2^T\mathbf{y}$$

- the orthogonal projector and orthogonal complement projector of $\mathbf{A}$ are resp. defined as

$$\mathbf{P}_\mathbf{A} = \mathbf{U}_1\mathbf{U}_1^T, \qquad \mathbf{P}_\mathbf{A}^\perp = \mathbf{U}_2\mathbf{U}_2^T$$

- properties (easy to show):
  - $\mathbf{P}_\mathbf{A}$ is idempotent, i.e., $\mathbf{P}_\mathbf{A}\mathbf{P}_\mathbf{A} = \mathbf{P}_\mathbf{A}$
  - $\mathbf{P}_\mathbf{A}$ is symmetric
  - the eigenvalues of $\mathbf{P}_\mathbf{A}$ are either 0 or 1
  - $\mathcal{R}(\mathbf{P}_\mathbf{A}) = \mathcal{R}(\mathbf{A})$
  - the same properties above apply to $\mathbf{P}_\mathbf{A}^\perp$, and $\mathbf{I} = \mathbf{P}_\mathbf{A} + \mathbf{P}_\mathbf{A}^\perp$

Minimum 2-Norm Solution to Underdetermined Linear Systems

- consider solving the linear system $\mathbf{y} = \mathbf{A}\mathbf{x}$ when $\mathbf{A}$ is fat
- this is an underdetermined problem: we have more unknowns n than the number of equations m
- assume that $\mathbf{A}$ has full row rank. By now we know that any

$$\mathbf{x} = \mathbf{A}^\dagger \mathbf{y} + \boldsymbol{\eta}, \quad \boldsymbol{\eta} \in \mathcal{R}(\mathbf{V}_2)$$

  is a solution to $\mathbf{y} = \mathbf{A}\mathbf{x}$, but we may want to grab one solution only
- Idea: discard $\boldsymbol{\eta}$ and take $\mathbf{x} = \mathbf{A}^\dagger \mathbf{y}$ as our solution
- Question: does discarding $\boldsymbol{\eta}$ make sense?
- Answer: it makes sense under the minimum 2-norm problem formulation

$$\min_{\mathbf{x} \in \mathbb{R}^n} \ \|\mathbf{x}\|_2^2 \qquad \text{s.t. } \mathbf{y} = \mathbf{A}\mathbf{x}$$

  It can be shown that the solution is uniquely given by $\mathbf{x} = \mathbf{A}^\dagger \mathbf{y}$ (try the proof)

Low-Rank Matrix Approximation

Aim: given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and an integer k with $1 \leq k < \mathrm{rank}(\mathbf{A})$, find a matrix $\mathbf{B} \in \mathbb{R}^{m \times n}$ such that $\mathrm{rank}(\mathbf{B}) \leq k$ and $\mathbf{B}$ best approximates $\mathbf{A}$

- it is somehow unclear about what a best approximation means, and we will specify one later
- closely related to the matrix factorization problem considered in Lecture 2
- applications: PCA, dimensionality reduction,...—the same kind of applications in matrix factorization
- truncated SVD: denote

$$\mathbf{A}_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T.$$

  Perform the aforementioned approximation by choosing $\mathbf{B} = \mathbf{A}_k$

Toy Application Example: Image Compression

- let $\mathbf{A} \in \mathbb{R}^{m \times n}$ be a matrix whose (i,j)th entry a_{ij} stores the (i,j)th pixel of an image.

- memory size for storing $\mathbf{A}$: mn

- truncated SVD: store $\{\mathbf{u}_i, \sigma_i \mathbf{v}_i\}_{i=1}^k$ instead of the full $\mathbf{A}$, and recover the image by $\mathbf{B} = \mathbf{A}_k$

- memory size for truncated SVD: $(m+n)k$
  - much less than mn if $k \ll \min\{m,n\}$

Toy Application Example: Image Compression

(a) original image, size= 102×1347

(b) truncated SVD, k= 5

(c) truncated SVD, k= 10

(d) truncated SVD, k= 20

Low-Rank Matrix Approximation

- truncated SVD provides the best approximation in the LS sense:

  Theorem 5.3 (Eckart-Young-Mirsky)**.** Consider the following problem

$$\min_{\mathbf{B} \in \mathbb{R}^{m \times n},\ \text{rank}(\mathbf{B}) \leq k} \|\mathbf{A} - \mathbf{B}\|_F^2$$

  where $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $k \in \{1, \ldots, p\}$ are given. The truncated SVD $\mathbf{A}_k$ is an optimal solution to the above problem.

- also note the matrix 2-norm version of the Eckart-Young-Mirsky theorem:

  Theorem 5.4. Consider the following problem

$$\min_{\mathbf{B} \in \mathbb{R}^{m \times n},\ \text{rank}(\mathbf{B}) \leq k} \|\mathbf{A} - \mathbf{B}\|_2$$

  where $\mathbf{A} \in \mathbb{R}^{m \times n}$ and $k \in \{1, \ldots, p\}$ are given. The truncated SVD $\mathbf{A}_k$ is an optimal solution to the above problem.

Low-Rank Matrix Approximation

- recall the matrix factorization problem in Lecture 2:

$$\min_{\mathbf{A}\in\mathbb{R}^{m\times k},\mathbf{B}\in\mathbb{R}^{k\times n}} \|\mathbf{Y}-\mathbf{A}\mathbf{B}\|_F^2$$

where $k \leq \min\{m,n\}$; $\mathbf{A}$ denotes a basis matrix; $\mathbf{B}$ is the coefficient matrix

- the matrix factorizaton problem may be reformulated as (verify)

$$\min_{\mathbf{Z}\in\mathbb{R}^{m\times n},\mathrm{rank}(\mathbf{Z})\leq k} \|\mathbf{Y}-\mathbf{Z}\|_F^2,$$

and the truncated SVD $\mathbf{Y}_k = \sum_{i=1}^{k} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$, where $\mathbf{Y} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$ denotes the SVD of $\mathbf{Y}$, is an optimal solution by Theorem 5.4

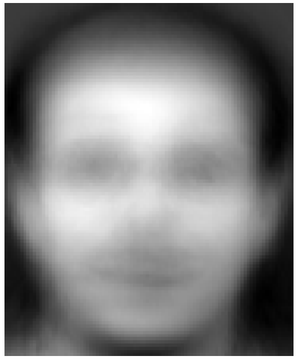
- thus, an optimal solution to the matrix factorization problem is

$$\mathbf{A} = [\ \mathbf{u}_1,\ldots,\mathbf{u}_k\ ], \qquad \mathbf{B} = [\ \sigma_1\mathbf{v}_1,\ldots,\sigma_k\mathbf{v}_k\ ]^T$$

Toy Demo: Dimensionality Reduction of a Face Image Dataset

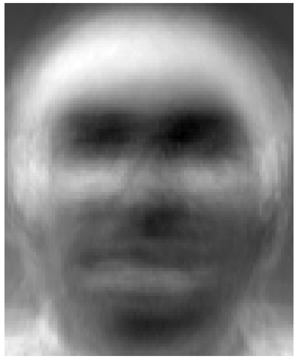
A face image dataset. Image size $= 112 \times 92$, number of face images $= 400$. Each $\mathbf{x}_i$ is the vectorization of one face image, leading to $m = 112 \times 92 = 10304$, $n = 400$.

Toy Demo: Dimensionality Reduction of a Face Image Dataset

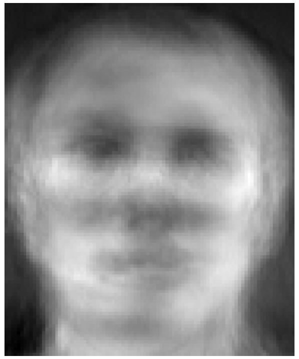


Mean face

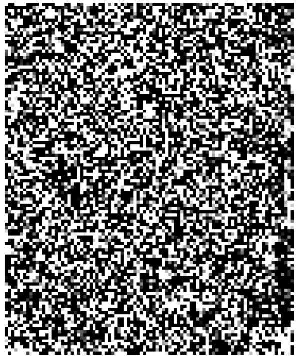
1st principal left singular vector



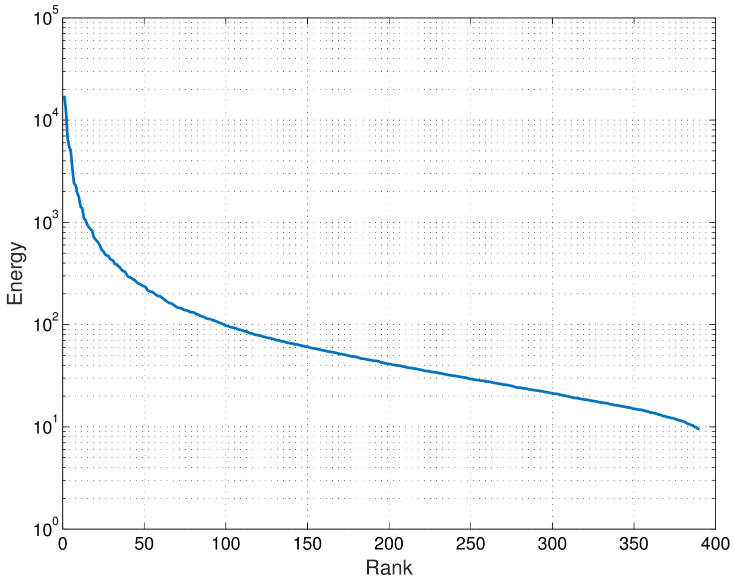
2nd principal left singular vector



3rd principal left singular vector



400th left singular vector



Energy Concentration

Singular Value Inequalities

Similar to variational characterization of eigenvalues of real symmetric matrices, we can derive various variational characterization results for singular values, e.g.,

- Courant-Fischer characterization:

$$\sigma_k(\mathbf{A}) = \min_{\dim \mathcal{S}_{n-k+1} \subseteq \mathbb{R}^n} \max_{\mathbf{x} \in \mathcal{S}_{n-k+1},\ \|\mathbf{x}\|_2 = 1} \|\mathbf{A}\mathbf{x}\|_2$$

- Weyl's inequality: for any $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{m \times n}$,

$$\sigma_{k+l-1}(\mathbf{A}+\mathbf{B}) \leq \sigma_k(\mathbf{A}) + \sigma_l(\mathbf{B}), \qquad k, l \in \{1, \ldots, p\},\ k+l-1 \leq p.$$

  Also, note the corollaries

  - $\sigma_k(\mathbf{A}+\mathbf{B}) \leq \sigma_k(\mathbf{A}) + \sigma_1(\mathbf{B})$, $k = 1, \ldots, p$
  - $|\sigma_k(\mathbf{A}+\mathbf{B}) - \sigma_k(\mathbf{A})| \leq \sigma_1(\mathbf{B})$, $k = 1, \ldots, p$

- and many more...

Proof of the Eckart-Young-Mirsky Thm. by Weyl's Inequality

An application of singular value inequalities is that of proving Theorem 5.4:

- for any $\mathbf{B}$ with $\mathrm{rank}(\mathbf{B}) \leq k$, we have
  - $\sigma_l(\mathbf{B}) = 0$ for $l > k$
  - (Weyl) $\sigma_{i+k}(\mathbf{A}) \leq \sigma_i(\mathbf{A} - \mathbf{B}) + \sigma_{k+1}(\mathbf{B}) = \sigma_i(\mathbf{A} - \mathbf{B})$ for $i = 1, \ldots, p - k$
  - and consequently

$$\|\mathbf{A} - \mathbf{B}\|_F^2 = \sum_{i=1}^{p} \sigma_i(\mathbf{A} - \mathbf{B})^2 \geq \sum_{i=1}^{p-k} \sigma_i(\mathbf{A} - \mathbf{B})^2 \geq \sum_{i=k+1}^{p} \sigma_i(\mathbf{A})^2$$

- the equality above is attained if we choose $\mathbf{B} = \mathbf{A}_k$

Computing the SVD via the Power Method

The power method can be used to compute the thin SVD, and the idea is as follows.

- assume $m \geq n$ and $\sigma_1 > \sigma_2 > \ldots \sigma_n > 0$
- apply the power method to $\mathbf{A}^T\mathbf{A}$ to obtain $\mathbf{v}_1$
- obtain $\mathbf{u}_1 = \mathbf{A}\mathbf{v}_1/\|\mathbf{A}\mathbf{v}_1\|_2, \sigma_1 = \|\mathbf{A}\mathbf{v}_1\|_2$ (why is this true?)
- do deflation $\mathbf{A} := \mathbf{A} - \sigma_1\mathbf{u}_1\mathbf{v}_1^T$, and repeat the above steps until all singular components are found

References

[Recht-Fazel-Parrilo'10] B. Recht, M. Fazel, and P. A. Parrilo, "Guaranteed minimum-rank solutions of linear matrix equations via nuclear norm minimization," *SIAM Review*, vol. 52, no. 3, pp. 471–501, 2010.