SINGULAR VALUE DECOMPOSITION

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LOGISTICS

General announcements

- Assignment 6 to be posted... (grading traffic jam)
- 7 lectures left!

Assignment 5 and Midterm 2:

Grading starting, we'll keep you posted

2/22

Last time:

Singular value decomposition

Today

Application to solving least squares

Reading: lecture notes 13/14



Toddlers can do it!

SINGULAR VALUE DECOMPOSITION

What happens for non-square matrice?

Theorem (Singular value decomposition)

Let $\mathbf{A} \in \mathbb{R}^{m imes n}$ with $\mathrm{rank}(\mathbf{A}) = r$. Then $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ where

- $\mathbf{U} \in \mathbb{R}^{m \times r}$ such that $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}_r$ (orthonormal columns) $(\mathcal{V}\mathcal{I}_{\#}^{\mathsf{T}}\mathbf{I})$ $\mathcal{U}_{=} [\mathcal{V}_{*}^{\mathsf{T}}\mathcal{I}_{*}]$ $\mathcal{U}_{=} [\mathcal{V}_{*}^{\mathsf{T}}\mathcal{I}_{*}]$
- $\mathbf{V} \in \mathbb{R}^{n \times r}$ such that $\mathbf{V}^{\intercal} \mathbf{V} = \mathbf{I}_r$ (orthonormal columns)
- $\Sigma \in \mathbb{R}^{r \times r}$ is diagonal with *positive entries*

$$oldsymbol{\Sigma} riangleq egin{bmatrix} \sigma_1 & 0 & 0 & \cdots \ 0 & \sigma_2 & 0 & \cdots \ dots & dots &$$

 $(\forall v^{\top} \neq I)$

and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r \geq 0$. The σ_i are called the singular values

We say that **A** is full rank is $r = \min(m, n)$

We can write $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\mathsf{T}}$









The vectors
$$\{u_i\}_{i=1}^{r}$$
 from a basis for the column space of A
Check: let's consider the span of $\{u_i\}_{i=1}^{r}$; note that $\forall c \in [i_jr] \; u_i \stackrel{\circ}{=} \stackrel{1}{\underset{l=1}{l}} A v_i \in c$
By dimension considerations dim (span $\{u_i\}_{i=1}^{r}\} = r = rank(A) = dom(cd(A))$ so that
Let $\{u_i\}_{i=r_1}^{m}$ be an althobass of Ken (A^T) ; recall that $Ken(A^T) = Gl(A)^L$ (check
Hence $\{u_i\}_{i=1}^{m}$ form an althobass for \mathbb{R}^m
Recall: $V \stackrel{\circ}{=} \begin{bmatrix} v_1 \cdots v_r \\ 1 & \cdots & v_r \end{bmatrix}$
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 $U \stackrel{\circ}{=} [u_1 \cdots u_r]$
 $U \stackrel{\circ}{=} I \quad U \stackrel{\circ}{=} U \stackrel{$

Compute
$$(U_{i}AV_{i})_{ij} = U_{i}Av_{i} = \frac{1}{14c}v_{i}AAv_{i} = The v_{i}V_{i}v_{j} = \begin{cases} di & if i=0 \\ 0 & else \end{cases}$$

Hence $U_{i}AV_{i} = \begin{bmatrix} U_{i} & 0 & 0 \\ 0 & U_{i}AV_{i} & 0 & 0 \\ 0 & U_{i}AV_{i}$

cd (A) so that span {uising C col(A) at span {uising = Col(A) k using definition + dimension}

- $\sqrt[4]{V_0} = 0$ $U^{T_0} = 0$
- /=W^T=I
- IV, ERMXN)

Prof. Shed with
$$A^{T}A \in \mathbb{R}^{n \times n}$$
, which is symmetric
By the spectral theorem, we have $A^{T}_{A} = \sum_{i=1}^{n} \lambda_{i} \vee_{i} \vee_{i}^{T}$ $\{V_{i}\}_{i=1}^{n}$ of the basis of A^{T}_{i}
Note that rank $(A) = \operatorname{rank}(A^{T}_{A}) = r \leq n$ so that $\lambda_{1} > \lambda_{2} - ... > \lambda_{r} > 0 = \lambda_{r}$
Consider $\{v_{i}\}_{i=1}^{r}$; they from an othobasis for the column space of (A^{T}_{A}) , hence of
Consider $\{v_{i}\}_{i=1}^{n}$; they from an othobasis for the kennel (mill space) of A^{T}_{A}
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Consider $\{v_{i}\}_{i=1}^{n}$; they form an othobasis for the kennel (mill space) of A^{T}_{A}
Consider $\{v_{i}\}_{i=1}^{n}$; they form $A^{T}_{A} = 0$ for $i \in I[r+1; n]$
Hence $\forall_{i} \in Ken(A^{T}_{A}) = Ken(A)$; $Span \{v_{i}\}_{i=r+1}^{n} \subset Ken(A)$
 (a) We have a span of dimension $n-r$ and $\dim(Ken(A)) = n-$ can be
Set $v_{i} = \frac{1}{|A|} A^{T}_{A}$ for $i \in I[1;r]$; form $U = [v_{i}]_{i=1}^{n} \sqrt{v_{i}} Y_{i} = [1]_{i=1}^{n}$
Note that $v_{i}v_{i} = \frac{1}{|A|} A^{T}_{A} = \frac{1}{$





IMPORTANT PROPERTIES OF THE SVD

The columns of $\mathbf{V} \{\mathbf{v}_i\}_{i=1}^r$ are eigenvectors of the psd matrix $\mathbf{A}^{\intercal} \mathbf{A}$. $\{\sigma_i : 1 \leq i \leq n \text{ and } \sigma_i \neq 0\}$ are the square roots of the non-zero eigenvalues of $\mathbf{A}^{\mathsf{T}}\mathbf{A}$.

Note: Since A=UZV ATA=VZUTUZV=VZVT



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The columns of $\mathbf{U} \{\mathbf{u}_i\}_{i=1}^r$ are eigenvectors of the psd matrix $\mathbf{A}\mathbf{A}^\intercal$. $\{\sigma_i : 1 \le i \le n \text{ and } \sigma_i \ne 0\}$ are the square roots of the non-zero eigenvalues of AA^{T} .



IMPORTANT PROPERTIES OF THE SVD

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The columns of $\mathbf{U} \{\mathbf{u}_i\}_{i=1}^r$ are eigenvectors of the psd matrix $\mathbf{A}\mathbf{A}^\intercal$. $\{\sigma_i : 1 \le i \le n \text{ and } \sigma_i \ne 0\}$ are the square roots of the non-zero eigenvalues of $\mathbf{A}\mathbf{A}^{\mathsf{T}}$.

The columns of V form an orthobasis for row(A)

The columns of \mathbf{U} form an orthobasis for $\mathrm{col}(\mathbf{A})$

Equivalent form of the SVD: $\mathbf{A} = \widetilde{\mathbf{U}} \widetilde{\mathbf{\Sigma}} \widetilde{\mathbf{V}}^T$ where

- $\widetilde{\mathbf{U}} \in \mathbb{R}^{m \times m}$ is orthonormal
- $\widetilde{\mathbf{V}} \in \mathbb{R}^{n \times n}$ is orthonormal
- $\widetilde{\mathbf{\Sigma}} \in \mathbb{R}^{m \times n}$ is

$$\widetilde{\boldsymbol{\Sigma}} \triangleq \begin{bmatrix} \boldsymbol{\Sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} \end{bmatrix}$$



SVD AND LEAST-SQUARES

When we cannot solve $\mathbf{y} = \mathbf{A}\mathbf{x}$, we solve instead

$$\min_{\mathbf{x} \in \mathbb{R}^n} ||\mathbf{x}||_2^2 \text{ such that } \mathbf{A}^\mathsf{T} \mathbf{A} \mathbf{x} = \mathbf{A}^\mathsf{T} \mathbf{y}$$

• This allows us to pick the minimum norm solution among potentially infinitely many solutions of the normal equations.

Recall: when $\mathbf{A} \in \mathbb{R}^{m imes n}$ is of rank n, then $\mathbf{x} = \mathbf{A}^\intercal (\mathbf{A} \mathbf{A}^\intercal)^{-1} \mathbf{y}$

Proposition (General solution) The solution of

$$\min_{\mathbf{x} \in \mathbb{R}^n} \| \, \mathbf{x} \|_2^2 \text{ such that } \mathbf{A}^\mathsf{T} \mathbf{A} \mathbf{x} = \mathbf{A}^\mathsf{T} \mathbf{y}$$

is

$$\hat{\mathbf{x}} = \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{U}^{\mathsf{T}} \mathbf{y} = \sum_{i=1}^{r} \frac{1}{\sigma_i} \langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i$$

where $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ is the SVD of \mathbf{A} .

in SVD analysis

12 + 11 Voda 12 = dTV Vd + dTVJ Vodo $= \| \chi \|_{2}^{2} + \| \chi \|_{2}^{2}$

+U(B-ZX)

PSEUDO INVERSE

 $\mathbf{A}^+ = \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{U}^{\mathsf{T}}$ is called the *pseudo-inverse*, Lanczos inverse, or Moore-Penrose inverse of $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$.

If **A** is square invertible then $\mathbf{A}^+ = \mathbf{A}$

If $m \geq n$ (tall and skinny matrix) of rank n then $\mathbf{A}^+ = (\mathbf{A}^\intercal \mathbf{A})^{-1} \mathbf{A}^\intercal$

If $m \geq m$ (short and fat matrix) of rank m then $\mathbf{A}^+ = \mathbf{A}^\intercal (\mathbf{A} \mathbf{A}^\intercal)^{-1}$

Note A^+ is as "close" to an inverse of A as possible

STABILITY OF LEAST SQUARES

What if we observe $\mathbf{y} = \mathbf{A}\mathbf{x}_0 + \mathbf{e}$ and we apply the pseudo inverse? $\hat{\mathbf{x}} = \mathbf{A}^+\mathbf{y}$ We can separate the error analysis into two components

$$\hat{\mathbf{x}} - \mathbf{x}_0 = \underbrace{\mathbf{A}^+ \mathbf{A} \mathbf{x}_0 - \mathbf{x}_0}_{\text{null space error}} + \underbrace{\mathbf{A}^+ \mathbf{e}}_{\text{noise error}}$$

$$= A^+ g - \mathbf{x}_0 = A^+ (A \mathbf{x}_0 + \mathbf{e}) - \mathbf{x}_0$$
Note $A^+ A \mathbf{x}_0 = \mathbf{V} \cdot \mathbf{\Sigma}^- \mathbf{U} \mathbf{U} \cdot \mathbf{\Sigma} \mathbf{V}^\top \mathbf{x}_0 = \mathbf{V} \mathbf{V}^\top \mathbf{x}_0 \neq \mathbf{T} \mathbf{x}_0$ in general, which means thet
$$(\text{when rank}(A) < n, \text{ i.e. Ker}(A) \text{ non trained}$$

we don't reconstruct to exactly al)

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We will express the error in terms of the SVD $\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathsf{T}}$ With

- $\{\mathbf{v}_i\}_{i=1}^r$ orthobasis of $\operatorname{row}(\mathbf{A})$, augmented by $\{\mathbf{v}_i\}_{i=1}^{r+1} \in \ker \mathbf{A}$ to form an orthobasis of \mathbb{R}^n
- $\{\mathbf{u}_i\}_{i=1}^r$ orthobasis of $\operatorname{col}(\mathbf{A})$, augmented by $\{\mathbf{u}\}_{i=1}^{r+1} \in \ker \mathbf{A}^{\mathsf{T}}$ to form an orthobasis of \mathbb{R}^m

The null space error is given by

$$\left\|\mathbf{A}^{+}\mathbf{A}\mathbf{x}_{0}-\mathbf{x}_{0}
ight\|_{2}^{2}=\sum_{i=r+1}^{n}\left|\langle\mathbf{v}_{i},oldsymbol{x}_{0}
ight
angle
ight|^{2}$$

Note:

$$X_{0} = \sum_{i=1}^{n} \langle x_{0i} \rangle_{i} > V_{i} = \sum_{i=1}^{r} \langle x_{0i} \rangle_{i} > V_{i} + \sum_{i=r+1}^{n} \langle x_{0i} \rangle_{i} > V_{i}$$

$$= \bigvee_{i=1}^{r} \bigvee_{i} \bigvee_{i} \bigvee_{i} \bigvee_{i} \rangle_{i} = \bigvee_{i=r+1}^{n} \bigvee_{i} \bigvee_{i} \bigvee_{i} \bigvee_{i} \bigvee_{i} \bigvee_{i} \rangle_{i}$$

$$= A^{\dagger}A \times_{0}$$

$$(|A^{\dagger}A \times_{0} - x_{0}||_{2}^{Z} = \sum_{i=1}^{n} |\langle x_{0i} \rangle_{i} > |^{Z}$$

STABILITY OF LEAST SQUARES

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The null space error is given by

$$ig\|\mathbf{A}^+\mathbf{A}\mathbf{x}_0-\mathbf{x}_0ig\|_2^2 = \sum_{i=r+1}^n |\langle \mathbf{v}_i,x_0
angle|^2$$

The noise error is given by

$$ig\|\mathbf{A}^+\mathbf{e}ig\|_2^2 = \sum_{i=1}^r \underbrace{rac{1}{\sigma_i^2}}_{i} |\langle\!\langle \mathbf{e}, \mathbf{u}_i
angle|^2$$

$$A^{\dagger}e = V Z^{-1} U e = \sum_{i=1}^{r} \frac{1}{\nabla_{i}} v_{i} v_{i} e = \sum_{i=1}^{r} \frac{1}{\nabla_{i}} \langle v_{i} e \rangle v_{i}$$

$$\|A^{\dagger}e\|_{L}^{2} = \sum_{i=1}^{r} \frac{1}{\nabla_{i}^{2}} |\langle v_{i} e \rangle|^{2}$$

STABLE RECONSTRUCTION BY TRUNCATION

How do we mitigate the effect of small singular values in reconstruction?

$$\hat{\mathbf{x}} = \mathbf{V} \mathbf{\Sigma}^{-1} \mathbf{U}^{\mathsf{T}} \mathbf{y} = \sum_{i=1}^{r} \frac{1}{\sigma_i} \langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i$$

Truncate the SVD to $r^\prime < r$

$$\mathbf{A}_t riangleq \sum_{i=1}^{r'} \sigma_i \mathbf{u}_i \mathbf{v}_i^{\intercal} \qquad \mathbf{A}_t^+ = \sum_{i=1}^{r'} rac{1}{\sigma_i} \mathbf{u}_i \mathbf{v}_i^{\intercal}$$

Reconstruct
$$\hat{\mathbf{x}}_t = \sum_{i=1}^{r'} \frac{1}{\sigma_i} \langle \mathbf{y}, \mathbf{u}_i \rangle \mathbf{v}_i = \mathbf{A}_t$$

Error analysis:

$$ig\| \hat{\mathbf{x}}_t ig\|_2^2 = \sum_{i=r+1}^n |\langle \mathbf{x}_0, \mathbf{v}_i
angle|^2 + \sum_{i=r'+1}^r |\langle \mathbf{x}_0, \mathbf{v}_i
angle|^2 + \sum_{i=1}^{r'} rac{1}{\sigma_i^2}$$

$rac{1}{2} |\langle \mathbf{e}, \mathbf{u}_i angle|^2$

STABLE RECONSTRUCTION BY REGULARIZATION

Regularization means changing the problem to solve

$$\min_{\mathbf{x}\in\mathbb{R}^n}\|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2+\lambda\|\mathbf{x}\|_2^2\qquad\lambda>0$$

The solution is

$$\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A} + \lambda\mathbf{I})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{y} = \mathbf{V}(\mathbf{\Sigma}^{2} + \lambda\mathbf{I})^{-1}\mathbf{\Sigma}\mathbf{U}$$





NUMERICAL METHODS

We have seen several solutions to systems of linear equations $\mathbf{A}\mathbf{x}=\mathbf{y}$ so far

- A full column rank: $\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{y}$
- A full row rank: $\hat{\mathbf{x}} = \mathbf{A}^{\mathsf{T}} (\mathbf{A} \mathbf{A}^{\mathsf{T}})^{-1} \mathbf{y}$
- Ridge regression: $\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A} + \delta\mathbf{I})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{y}$
- Kernel regression: $\hat{\mathbf{x}} = (\mathbf{K} + \delta \mathbf{I})^{-1} \mathbf{y}$
- Ridge regression in Hilbert space: $\hat{\mathbf{x}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A} + \delta\mathbf{G})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{y}$

Extension: constrained least-squares

$$\min_{\mathbf{x}\in\mathbb{R}^n}\|\mathbf{y}-\mathbf{A}\mathbf{x}\|_2^2 ext{ s.t. } \mathbf{x} = \mathbf{B}oldsymbollpha ext{ for some }oldsymbollpha$$

• The solution is $\hat{\mathbf{x}} = \mathbf{B} (\mathbf{B}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{A} \mathbf{B})^{-1} \mathbf{B}^{\mathsf{T}} \mathbf{A}^{\mathsf{T}} \mathbf{y}$

All these problems involve a symmetric positive definite system of equations.

Many methods to achieve this based on matrix factorization

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EASY SYSTEMS

Diagonal system

- $\mathbf{A} \in \mathbb{R}^{n imes n}$ invertible and diagonal
- O(n) complexity

Orthogonal system

- $\mathbf{A} \in \mathbb{R}^{n imes n}$ invertible and orthogonal
- $O(n^2)$ complexity

Lower triangular system

- $\mathbf{A} \in \mathbb{R}^{n imes n}$ invertible and lower diagonal
- $O(n^2)$ complexity

General strategy: factorize ${f A}$ to recover some of the structures above

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