4. Singular value decomposition

- singular value decomposition
- related eigendecompositions
- matrix properties from singular value decomposition
- min–max and max–min characterizations
- low-rank approximation
- sensitivity of linear equations

Singular value decomposition (SVD)

every $m \times n$ matrix A can be factored as

$$A = U\Sigma V^T$$

- U is $m \times m$ and orthogonal
- V is $n \times n$ and orthogonal
- Σ is $m \times n$ and "diagonal": diagonal with diagonal elements $\sigma_1, \ldots, \sigma_n$ if $m = n$,

$$\Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_n \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} \quad \text{if } m > n, \qquad \Sigma = \begin{bmatrix} \sigma_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \sigma_m & 0 & \cdots & 0 \end{bmatrix} \quad \text{if } m < n$$

- the diagonal entries of Σ are nonnegative and sorted:

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min\{m,n\}} \geq 0$$

Singular values and singular vectors

$$A = U\Sigma V^T$$

- the numbers $\sigma_1, \ldots, \sigma_{\min\{m,n\}}$ are the *singular values* of A
- the m columns u_i of U are the *left singular vectors*
- the n columns v_i of V are the *right singular vectors*

if we write the factorization $A = U\Sigma V^T$ as

$$AV = U\Sigma, \qquad A^T U = V\Sigma^T$$

and compare the ith columns on the left- and right-hand sides, we see that

$$Av_i = \sigma_i u_i \quad \text{and} \quad A^T u_i = \sigma_i v_i \qquad \text{for } i = 1, \ldots, \min\{m, n\}$$

- if $m > n$ the additional $m - n$ vectors u_i satisfy $A^T u_i = 0$ for $i = n + 1, \ldots, m$
- if $n > m$ the additional $n - m$ vectors v_i satisfy $Av_i = 0$ for $i = m + 1, \ldots, n$

Reduced SVD

often $m \gg n$ or $n \gg m$, which makes one of the orthogonal matrices very large

Tall matrix: if $m > n$, the last $m - n$ columns of U can be omitted to define

$$A = U\Sigma V^T$$

- U is $m \times n$ with orthonormal columns
- V is $n \times n$ and orthogonal
- Σ is $n \times n$ and diagonal with diagonal entries $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \geq 0$

Wide matrix: if $m < n$, the last $n - m$ columns of V can be omitted to define

$$A = U\Sigma V^T$$

- U is $m \times m$ and orthogonal
- V is $m \times n$ with orthonormal columns
- Σ is $m \times m$ and diagonal with diagonal entries $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_m \geq 0$

we refer to these as *reduced* SVDs (and to the factorization on p. 4.2 as a *full* SVD)

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Eigendecomposition of Gram matrix

suppose A is an $m \times n$ matrix with full SVD

$$A = U\Sigma V^T$$

the SVD is related to the eigendecomposition of the Gram matrix $A^T A$:

$$A^T A = V\Sigma^T \Sigma V^T$$

- V is an orthogonal $n \times n$ matrix
- $\Sigma^T \Sigma$ is a diagonal $n \times n$ matrix with (non-increasing) diagonal elements

$$\sigma_1^2, \quad \sigma_2^2, \quad \ldots, \quad \sigma_{\min\{m,n\}}^2, \quad \underbrace{0, \quad 0, \quad \cdots, \quad 0}_{n - \min\{m,n\} \text{ times}}$$

- the n diagonal elements of $\Sigma^T \Sigma$ are the eigenvalues of $A^T A$
- the right singular vectors (columns of V) are corresponding eigenvectors

Gram matrix of transpose

the SVD also gives the eigendecomposition of AA^T:

$$AA^T = U\Sigma\Sigma^T U^T$$

- U is an orthogonal $m \times m$ matrix
- $\Sigma\Sigma^T$ is a diagonal $m \times m$ matrix with (non-increasing) diagonal elements

$$\sigma_1^2, \quad \sigma_2^2, \quad \ldots, \quad \sigma_{\min\{m,n\}}^2, \quad \underbrace{0, \quad 0, \quad \cdots, \quad 0}_{m - \min\{m,n\} \text{ times}}$$

- the m diagonal elements of $\Sigma\Sigma^T$ are the eigenvalues of AA^T
- the left singular vectors (columns of U) are corresponding eigenvectors

in particular, the first $\min\{m,n\}$ eigenvalues of A^TA and AA^T are the same:

$$\sigma_1^2, \quad \sigma_2^2, \quad \ldots, \quad \sigma_{\min\{m,n\}}^2$$

Example

scatter plot shows $m = 500$ points from the normal distribution on page 3.34

$$\mu = \begin{bmatrix} 5 \\ 4 \end{bmatrix}, \qquad \Sigma_{\mathrm{ex}} = \frac{1}{4}\begin{bmatrix} 7 & \sqrt{3} \\ \sqrt{3} & 5 \end{bmatrix}$$

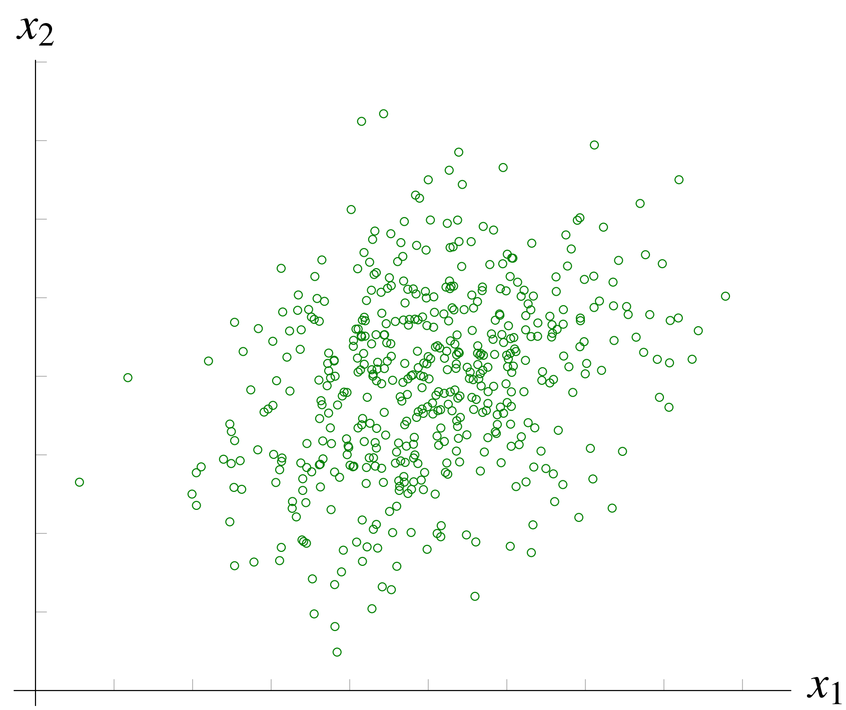
- we define an $m \times 2$ data matrix X with the m vectors as its rows
- the centered data matrix is $X_{\mathrm{c}} = X - (1/m)\mathbf{1}\mathbf{1}^T X$

sample estimate of mean is

$$\widehat{\mu} = \frac{1}{m}X^T\mathbf{1} = \begin{bmatrix} 5.01 \\ 3.93 \end{bmatrix}$$

sample estimate of covariance is

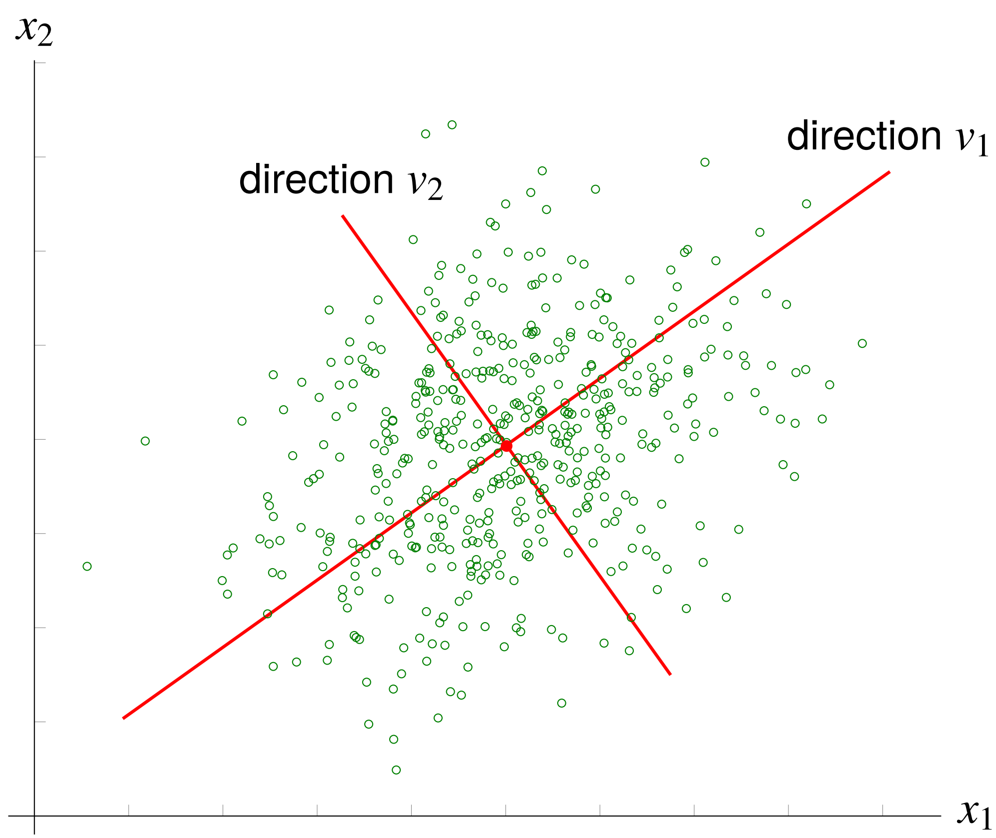
$$\widehat{\Sigma} = \frac{1}{m}X_{\mathrm{c}}^T X_{\mathrm{c}} = \begin{bmatrix} 1.67 & 0.48 \\ 0.48 & 1.35 \end{bmatrix}$$



Example

$$A = \frac{1}{\sqrt{m}} X_{\mathrm{c}}$$

- eigenvectors of $\widehat{\Sigma}$ are right singular vectors v_1, v_2 of A (and of X_{c})
- eigenvalues of $\widehat{\Sigma}$ are squares of the singular values of A



Existence of singular value decomposition

the Gram matrix connection gives a proof that every matrix has an SVD

- assume A is $m \times n$ with $m \geq n$ and rank r
- the $n \times n$ matrix $A^T A$ has rank r (page 2.5) and an eigendecomposition

$$A^T A = V \Lambda V^T \qquad (1)$$

  Λ is diagonal with diagonal elements $\lambda_1 \geq \cdots \geq \lambda_r > 0 = \lambda_{r+1} = \cdots = \lambda_n$

- define $\sigma_i = \sqrt{\lambda_i}$ for $i = 1, \ldots, n$, and an $n \times n$ matrix

$$U = \begin{bmatrix} u_1 & \cdots & u_n \end{bmatrix} = \begin{bmatrix} \frac{1}{\sigma_1} A v_1 & \frac{1}{\sigma_2} A v_2 & \cdots & \frac{1}{\sigma_r} A v_r & u_{r+1} & \cdots & u_n \end{bmatrix}$$

  where $u_{r+1}, \ldots, u_n$ form any orthonormal basis for $\operatorname{null}(A^T)$

- (1) and the choice of $u_{r+1}, \ldots, u_n$ imply that U is orthogonal
- (1) also implies that $A v_i = 0$ for $i = r+1, \ldots, n$
- together with the definition of $u_1, \ldots, u_r$ this shows that $AV = U\Sigma$

Non-uniqueness of singular value decomposition

the derivation from the eigendecomposition

$$A^T A = V \Lambda V^T$$

shows that the singular value decomposition of A is almost unique

Singular values

- the singular values of A are uniquely defined
- we have also shown that A and A^T have the same singular values

Singular vectors (assuming $m \geq n$): see the discussion on page 3.14

- right singular vectors v_i with the same positive singular value span a subspace
- in this subspace, any other orthonormal basis can be chosen
- the first $r = \text{rank}(A)$ left singular vectors then follow from $\sigma_i u_i = A v_i$
- the remaining vectors $v_{r+1}, \ldots, v_n$ can be any orthonormal basis for $\text{null}(A)$
- the remaining vectors $u_{r+1}, \ldots, u_m$ can be any orthonormal basis for $\text{null}(A^T)$

Exercise

suppose A is an $m \times n$ matrix with $m \geq n$, and define

$$B = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix}$$

1. suppose $A = U\Sigma V^T$ is a full SVD of A; verify that

$$B = \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} 0 & \Sigma \\ \Sigma^T & 0 \end{bmatrix} \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix}^T$$

2. derive from this an eigendecomposition of B

   Hint: if Σ_1 is square, then

$$\begin{bmatrix} 0 & \Sigma_1 \\ \Sigma_1 & 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} I & I \\ I & -I \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & -\Sigma_1 \end{bmatrix} \begin{bmatrix} I & I \\ I & -I \end{bmatrix}$$

3. what are the $m + n$ eigenvalues of B?

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Rank

the number of positive singular values is the rank of a matrix

- suppose there are r positive singular values:

$$\sigma_1 \geq \cdots \geq \sigma_r > 0 = \sigma_{r+1} = \cdots = \sigma_{\min\{m,n\}}$$

- partition the matrices in a full SVD of A as

$$\begin{aligned} A &= \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T \\ &= U_1 \Sigma_1 V_1^T \end{aligned} \tag{2}$$

  Σ_1 is $r \times r$ with the positive singular values $\sigma_1, \ldots, \sigma_r$ on the diagonal

- since U_1 and V_1 have orthonormal columns, the factorization (2) proves that

$$\text{rank}(A) = r$$

  (see page 1.12)

Inverse and pseudo-inverse

we use the same notation as on the previous page

$$A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T = U_1 \Sigma_1 V_1^T$$

diagonal entries of Σ_1 are the positive singular values of A

- pseudo-inverse follows from page 1.36:

$$\begin{aligned} A^\dagger &= V_1 \Sigma_1^{-1} U_1^T \\ &= \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} U_1^T \\ U_2^T \end{bmatrix} \\ &= V \Sigma^\dagger U^T \end{aligned}$$

- if A is square and nonsingular, this reduces to the inverse

$$A^{-1} = (U \Sigma V^T)^{-1} = V \Sigma^{-1} U^T$$

Four subspaces

we continue with the same notation for the SVD of an $m \times n$ matrix A with rank r:

$$A = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_1 & V_2 \end{bmatrix}^T$$

the diagonal entries of Σ_1 are the positive singular values of A

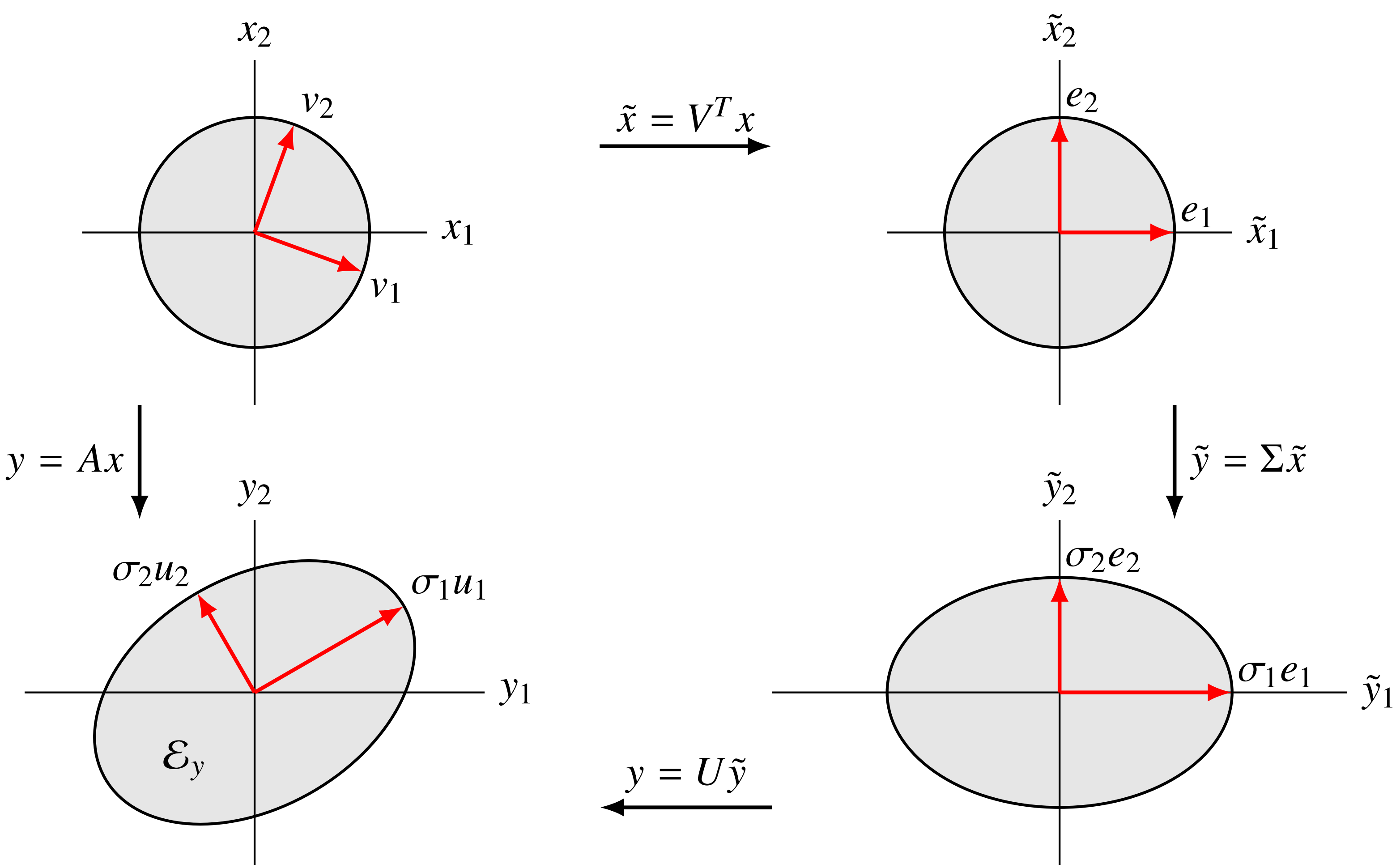
the SVD provides orthonormal bases for the four subspaces associated with A

- the columns of the $m \times r$ matrix U_1 are a basis of $\mathrm{range}(A)$
- the columns of the $m \times (m - r)$ matrix U_2 are a basis of $\mathrm{range}(A)^\perp = \mathrm{null}(A^T)$
- the columns of the $n \times r$ matrix V_1 are a basis of $\mathrm{range}(A^T)$
- the columns of the $n \times (n - r)$ matrix V_2 are a basis of $\mathrm{null}(A)$

Image of unit ball

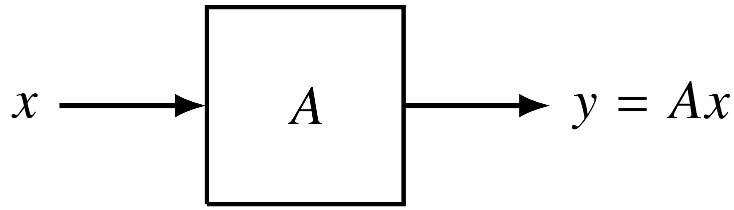
define $\mathcal{E}_y$ as the image of the unit ball under the linear mapping $y = Ax$:

$$\mathcal{E}_y = \{Ax \mid \|x\| \leq 1\} = \{U\Sigma V^T x \mid \|x\| \leq 1\}$$



Control interpretation

system A maps input x to output $y = Ax$



- if $\|x\|^2$ represents input energy, the set of outputs realizable with unit energy is

$$\mathcal{E}_y = \{Ax \mid \|x\| \leq 1\}$$

- assume $\mathrm{rank}(A) = m$: every desired y can be realized by at least one input
- the most energy-efficient input that generates output y is

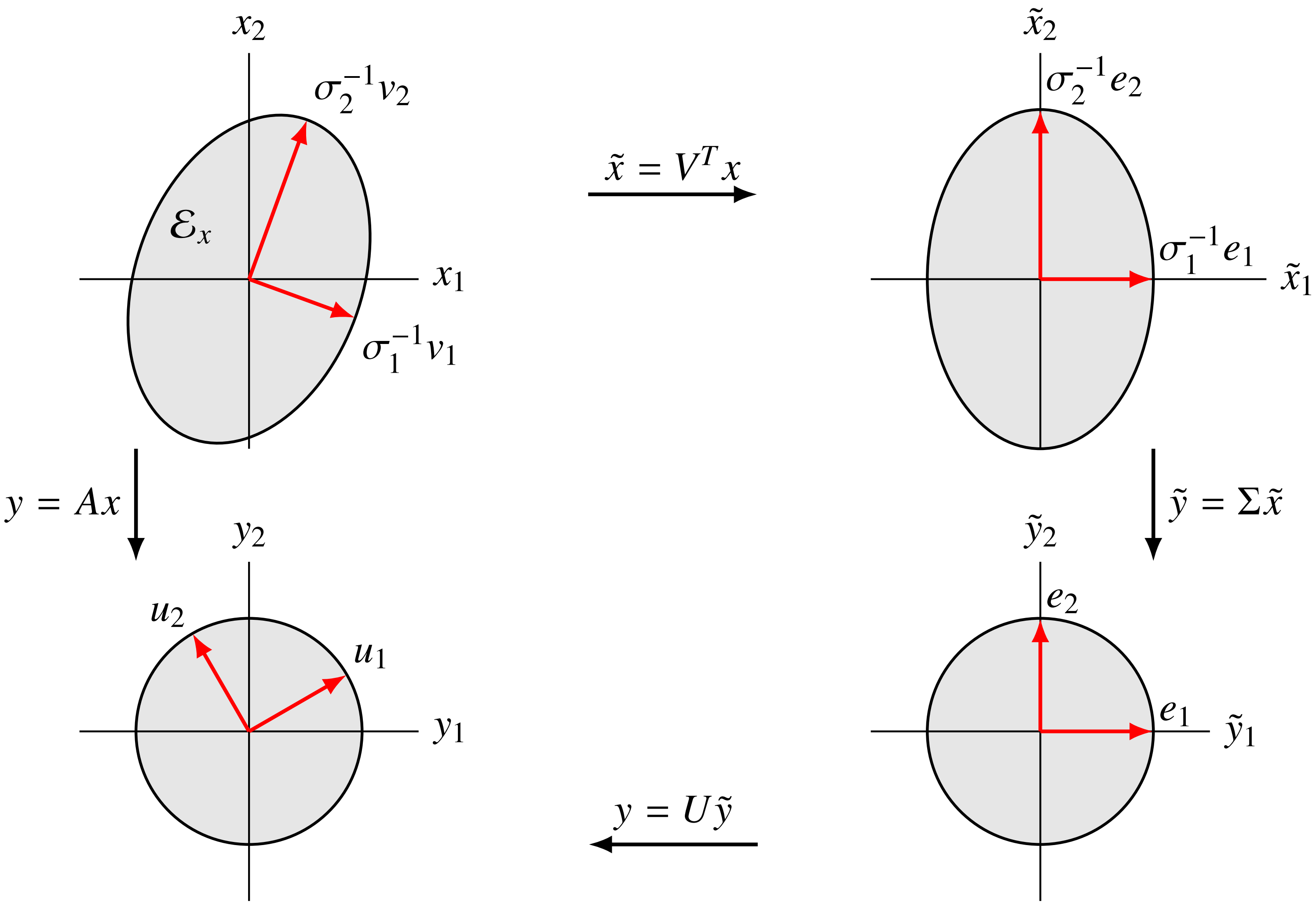
$$x_{\mathrm{eff}} = A^\dagger y = A^T(AA^T)^{-1}y, \qquad \|x_{\mathrm{eff}}\|^2 = y^T(AA^T)^{-1}y = \sum_{i=1}^{m} \frac{(u_i^T y)^2}{\sigma_i^2}$$

- (if $\mathrm{rank}(A) = m$) the set $\mathcal{E}_y$ is an ellipsoid $\mathcal{E}_y = \{y \mid y^T(AA^T)^{-1}y \leq 1\}$

Inverse image of unit ball

define $\mathcal{E}_x$ as the inverse image of the unit ball under the linear mapping $y = Ax$:

$$\mathcal{E}_x = \{x \mid \|Ax\| \leq 1\} = \{x \mid \|U\Sigma V^T x\| \leq 1\}$$



Estimation interpretation

measurement A maps unknown quantity x_{true} to observation

$$y_{\text{obs}} = A(x_{\text{true}} + v)$$

where v is unknown but bounded by $\|Av\| \leq 1$

- if $\operatorname{rank}(A) = n$, there is a unique estimate $\hat{x}$ that satisfies $A\hat{x} = y_{\text{obs}}$
- uncertainty in y causes uncertainty in estimate: true value x_{true} must satisfy

$$\|A(x_{\text{true}} - \hat{x})\| \leq 1$$

- the set $\mathcal{E}_x = \{x \mid \|A(x - \hat{x})\| \leq 1\}$ is the uncertainty region around estimate $\hat{x}$

Frobenius norm and 2-norm

for an $m \times n$ matrix A with singular values σ_i:

$$\|A\|_F = \left(\sum_{i=1}^{\min\{m,n\}} \sigma_i^2 \right)^{1/2}, \qquad \|A\|_2 = \sigma_1$$

this readily follows from the unitary invariance of the two norms:

$$\|A\|_F = \|U\Sigma V^T\|_F = \|\Sigma\|_F = \left(\sum_{i=1}^{\min\{m,n\}} \sigma_i^2 \right)^{1/2}$$

and

$$\|A\|_2 = \|U\Sigma V^T\|_2 = \|\Sigma\|_2 = \sigma_1$$

Exercise

Exercise 1: express $\|A^\dagger\|_2$ and $\|A^\dagger\|_F$ in terms of the singular values of A

Exercise 2: the condition number of a square nonsingular matrix A is defined as

$$\kappa(A) = \|A\|_2 \|A^{-1}\|_2$$

express $\kappa(A)$ in terms of the singular values of A

Exercise 3: give an SVD and the 2-norm of the matrix

$$A = ab^T$$

where a is an n-vector and b is an m-vector

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First singular value

the first singular value is the maximal value of several functions:

$$\sigma_1 = \max_{\|x\|=1} \|Ax\| = \max_{\|x\|=\|y\|=1} y^T A x = \max_{\|y\|=1} \|A^T y\| \tag{3}$$

- the first and last expressions follow from page 3.24 and

$$\sigma_1^2 = \lambda_{\max}(A^T A) = \max_{\|x\|=1} x^T A^T A x, \qquad \sigma_1^2 = \lambda_{\max}(A A^T) = \max_{\|y\|=1} y^T A A^T y$$

- second expression in (3) follows from the Cauchy–Schwarz inequality:

$$\|Ax\| = \max_{\|y\|=1} y^T (Ax), \qquad \|A^T y\| = \max_{\|x\|=1} x^T (A^T y)$$

First singular value

alternatively, we can use an SVD of A to solve the maximization problems in

$$\sigma_1 = \max_{\|x\|=1} \|Ax\| = \max_{\|x\|=\|y\|=1} y^T A x = \max_{\|y\|=1} \|A^T y\| \qquad (4)$$

- suppose $A = USV^T$ is a full SVD of A
- if we define $\tilde{x} = V^T x$, $\tilde{y} = U^T y$, then (4) can be written as

$$\sigma_1 = \max_{\|\tilde{x}\|=1} \|\Sigma \tilde{x}\| = \max_{\|\tilde{x}\|=\|\tilde{y}\|=1} \tilde{y}^T \Sigma \tilde{x} = \max_{\|\tilde{y}\|=1} \|\Sigma^T \tilde{y}\|$$

- an optimal choice for $\tilde{x}$ and $\tilde{y}$ is $\tilde{x} = (1, 0, \ldots, 0)$ and $\tilde{y} = (1, 0, \ldots, 0)$
- therefore $x = v_1$ and $y = u_1$ are optimal for each of the maximizations in (4)

Last singular value

two of the three expressions in (3) have a counterpart for the last singular value

- for an $m \times n$ matrix A, the last singular $\sigma_{\min\{m,n\}}$ can be written as follows:

$$\text{if } m \geq n: \quad \sigma_n = \min_{\|x\|=1} \|Ax\|, \qquad \text{if } n \geq m: \quad \sigma_m = \min_{\|y\|=1} \|A^T y\| \tag{5}$$

- if $m \neq n$, we need to distinguish the two cases because

$$\min_{\|x\|=1} \|Ax\| = 0 \quad \text{if } n > m, \qquad \min_{\|y\|=1} \|A^T y\| = 0 \quad \text{if } m > n$$

to prove (5), we substitute full SVD $A = U\Sigma V^T$, and define $\tilde{x} = V^T x$, $\tilde{y} = U^T y$:

$$\text{if } m \geq n: \qquad \min_{\|\tilde{x}\|=1} \|\Sigma \tilde{x}\| = \min_{\|\tilde{x}\|=1} \left(\sigma_1^2 \tilde{x}_1^2 + \cdots + \sigma_n^2 \tilde{x}_n^2\right)^{1/2} = \sigma_n$$

$$\text{if } n \geq m: \qquad \min_{\|\tilde{y}\|=1} \|\Sigma^T \tilde{y}\| = \min_{\|\tilde{y}\|=1} \left(\sigma_1^2 \tilde{y}_1^2 + \cdots + \sigma_m^2 \tilde{y}_m^2\right)^{1/2} = \sigma_m$$

optimal choices for x and y in (5) are $x = v_n$, $y = u_m$

Max–min characterization

we extend (3) to a max–min characterization of the other singular values:

$$\sigma_k = \max_{X^TX=I_k} \sigma_{\min}(AX) \tag{6a}$$

$$= \max_{X^TX=Y^TY=I_k} \sigma_{\min}(Y^TAX) \tag{6b}$$

$$= \max_{Y^TY=I_k} \sigma_{\min}(A^TY) \tag{6c}$$

- σ_k for $k = 1, \ldots, \min\{m, n\}$ are the singular values of the $m \times n$ matrix A
- X is $n \times k$ with orthonormal columns, Y is $m \times k$ with orthonormal columns
- $\sigma_{\min}(B)$ denotes the smallest singular value of the matrix B
- in the three expressions in (6) $\sigma_{\min}(\cdot)$ denotes the kth singular value
- for $k = 1$, we obtain the three expressions for σ_1 in (3)

- these can be derived from the min–max theorems for eigenvalues (p. 3.29)
- or we can find an optimal choice for X, Y from an SVD of A (we skip the details)

Min–max characterization

we extend (5) to a min–max characterization of all singular values

Tall or square matrix: if A is $m \times n$ with $m \geq n$

$$\sigma_{n-k+1} = \min_{X^T X = I_k} \|AX\|_2, \qquad k = 1, \ldots, n \tag{7}$$

- we minimize over $n \times k$ matrices X with orthonormal columns
- $\|AX\|_2$ is the maximum singular value of an $m \times k$ matrix
- for $k = 1$, this is the first expression in (5)

Wide or square matrix (A is $m \times n$ with $m \leq n$)

$$\sigma_{m-k+1} = \min_{Y^T Y = I_k} \|A^T Y\|_2, \qquad k = 1, \ldots, m$$

- we minimize over $n \times k$ matrices Y with orthonormal columns
- $\|A^T Y\|_2$ is the maximum singular value of an $n \times k$ matrix
- for $k = 1$, this is the second expression in (5)

Proof of min–max characterization (for $m \geq n$)

we use a full SVD $A = U\Sigma V^T$ to solve the optimization problem

$$\begin{array}{ll} \text{minimize} & \|AX\|_2 \\ \text{subject to} & X^T X = I \end{array}$$

changing variables to $\tilde{X} = V^T X$ gives the equivalent problem

$$\begin{array}{ll} \text{minimize} & \|\Sigma \tilde{X}\|_2 \\ \text{subject to} & \tilde{X}^T \tilde{X} = I \end{array}$$

- we show that the optimal value is σ_{n-k+1}
- an optimal solution for $\tilde{X}$ is formed from the last k columns of the $n \times n$ identity

$$\tilde{X}_{\text{opt}} = \left[\begin{array}{cccc} e_{n-k+1} & \cdots & e_{n-1} & e_n \end{array} \right]$$

- an optimal solution for X is formed from the last k columns of V:

$$X_{\text{opt}} = \left[\begin{array}{cccc} v_{n-k+1} & \cdots & v_{n-1} & v_n \end{array} \right]$$

Proof of min–max characterization (for $m \geq n$)

- we first note that $\Sigma \tilde{X}_{\text{opt}}$ are the last k columns of Σ, so $\|\Sigma \tilde{X}_{\text{opt}}\|_2 = \sigma_{n-k+1}$

- to show that this is optimal, consider any other $n \times k$ matrix $\tilde{X}$ with $\tilde{X}^T \tilde{X} = I$

- find a nonzero k-vector u for which $y = \tilde{X}u$ has last $k-1$ components zero:

$$\tilde{X}u = (y_1, \ldots, y_{n-k+1}, 0, \ldots, 0)$$

  this is possible because a $(k-1) \times k$ matrix has linearly dependent columns

- normalize u so that $\|u\| = \|y\| = 1$, and use it to lower bound $\|\Sigma \tilde{X}\|_2$:

$$\begin{aligned}
\|\Sigma \tilde{X}\|_2 &\geq \|\Sigma \tilde{X} u\|_2 \\
&= \|\Sigma y\|_2 \\
&= \left(\sigma_1^2 y_1^2 + \cdots + \sigma_{n-k+1}^2 y_{n-k+1}^2\right)^{1/2} \\
&\geq \sigma_{n-k+1} \left(y_1^2 + \cdots + y_{n-k+1}^2\right)^{1/2} \\
&= \sigma_{n-k+1}
\end{aligned}$$

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Rank-r approximation

let A be an $m \times n$ matrix with $\operatorname{rank}(A) > r$ and full SVD

$$A = U\Sigma V^T = \sum_{i=1}^{\min\{m,n\}} \sigma_i u_i v_i^T, \qquad \sigma_1 \geq \cdots \geq \sigma_{\min\{m,n\}} \geq 0, \quad \sigma_{r+1} > 0$$

the best rank-r approximation of A is the sum of the first r terms in the SVD:

$$B = \sum_{i=1}^{r} \sigma_i u_i v_i^T$$

- B is the best approximation for the Frobenius norm: for every C with rank r,

$$\|A - C\|_F \geq \|A - B\|_F = \left(\sum_{i=r+1}^{\min\{m,n\}} \sigma_i^2 \right)^{1/2}$$

- B is also the best approximation for the 2-norm: for every C with rank r,

$$\|A - C\|_2 \geq \|A - B\|_2 = \sigma_{r+1}$$

Rank-r approximation in Frobenius norm

the approximation problem in $\|\cdot\|_F$ is a nonlinear least squares problem:

$$\text{minimize} \quad \|A - YX^T\|_F^2 = \sum_{i=1}^{m}\sum_{j=1}^{n}\left(A_{ij} - \sum_{k=1}^{r} Y_{ik}X_{jk}\right)^2 \qquad (8)$$

- matrix B is written as $B = YX^T$ with Y of size $m \times r$ and X of size $n \times r$
- we optimize over X and Y

Outline of the solution

- the first order (necessary but not sufficient) optimality conditions are

$$AX = Y(X^TX), \qquad A^TY = X(Y^TY)$$

- can assume $X^TX = Y^TY = D$ with D diagonal (*e.g.*, get X, Y from SVD of B)
- then columns of X, Y are formed from r pairs of right/left singular vectors of A
- optimal choice for (8) is to take the first r singular vector pairs

Rank-r approximation in 2-norm

to show that B is the best approximation in 2-norm, we prove that

$$\|A - C\|_2 \geq \|A - B\|_2 \quad \text{for all } C \text{ with } \mathrm{rank}(C) = r$$

on the right-hand side

$$\begin{aligned}
A - B &= \sum_{i=1}^{\min\{m,n\}} \sigma_i u_i v_i^T - \sum_{i=1}^{r} \sigma_i u_i v_i^T \\
&= \sum_{i=r+1}^{\min\{m,n\}} \sigma_i u_i v_i^T \\
&= \left[\begin{array}{ccc} u_{r+1} & \cdots & u_{\min\{m,n\}} \end{array}\right] \left[\begin{array}{ccc} \sigma_{r+1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sigma_{\min\{m,n\}} \end{array}\right] \left[\begin{array}{ccc} v_{r+1} & \cdots & v_{\min\{m,n\}} \end{array}\right]^T
\end{aligned}$$

and the 2-norm of the difference is $\|A - B\|_2 = \sigma_{r+1}$

on the next page we show that $\|A - C\|_2 \geq \sigma_{r+1}$ if C has rank r

Proof: we prove that $\|A - C\|_2 \geq \sigma_{r+1}$ for all $m \times n$ matrices C of rank r

- we assume that $m \geq n$ (otherwise, first take the transpose of A and C)
- if $\mathrm{rank}(C) = r$, the nullspace of C has dimension $n - r$
- define an $n \times (n - r)$ matrix $\hat{X}$ with orthonormal columns that span $\mathrm{null}(C)$
- use the min–max characterization on page 4.25 to bound $\|A - C\|_2$:

$$
\begin{aligned}
\|A - C\|_2 &= \max_{\|x\|=1} \|(A - C)x\| \\
&\geq \max_{\|w\|=1} \|(A - C)\hat{X}w\| && (\|\hat{X}w\| = 1 \text{ if } \|w\| = 1) \\
&= \|(A - C)\hat{X}\|_2 \\
&= \|A\hat{X}\|_2 && (C\hat{X} = 0) \\
&\geq \min_{X^T X = I_{n-r}} \|AX\|_2 \\
&= \sigma_{r+1} && (\text{apply (7) with } k = n - r)
\end{aligned}
$$

Outline

- singular value decomposition
- related eigendecompositions
- matrix properties from singular value decomposition
- min–max and max–min characterizations
- low-rank approximation
- **sensitivity of linear equations**

SVD of square matrix

for the rest of the lecture we assume that A is $n \times n$ and nonsingular with SVD

$$A = U\Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T$$

- 2-norm of A is $\|A\|_2 = \sigma_1$
- A is nonsingular if and only if $\sigma_n > 0$
- inverse of A and 2-norm of A^{-1} are

$$A^{-1} = V\Sigma^{-1}U^T = \sum_{i=1}^{n} \frac{1}{\sigma_i} v_i u_i^T, \qquad \|A^{-1}\|_2 = \frac{1}{\sigma_n}$$

- condition number of A is

$$\kappa(A) = \|A\|_2 \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n} \geq 1$$

A is called *ill-conditioned* if the condition number is very high

Sensitivity to right-hand side perturbations

linear equation with right-hand side $b \neq 0$ and perturbed right-hand side $b + e$:

$$Ax = b, \qquad Ay = b + e$$

- bound on distance between the solutions:

$$\|y - x\| = \|A^{-1}e\| \leq \|A^{-1}\|_2 \|e\|$$

  recall that $\|Bx\| \leq \|B\|_2 \|x\|$ for matrix 2-norm and Euclidean vector norm

- bound on relative change in the solution, in terms of $\delta_b = \|e\|/\|b\|$:

$$\frac{\|y - x\|}{\|x\|} \leq \|A\|_2 \|A^{-1}\|_2 \frac{\|e\|}{\|b\|} = \kappa(A)\, \delta_b$$

  in the first step we use $\|b\| = \|Ax\| \leq \|A\|_2 \|x\|$

large $\kappa(A)$ indicates that the solution can be very sensitive to changes in b

Worst-case perturbation of right-hand side

$$\frac{\|y-x\|}{\|x\|} \leq \kappa(A)\,\delta_b \qquad \text{where } \delta_b = \frac{\|e\|}{\|b\|}$$

- the upper bound is often very conservative
- however, for every A one can find b, e for which the bound holds with equality

- choose $b = u_1$ (first left singular vector of A): solution of $Ax = b$ is

$$x = A^{-1}b = V\Sigma^{-1}U^T u_1 = \frac{1}{\sigma_1}v_1$$

- choose $e = \delta_b\, u_n$ (δ_b times left singular vector u_n): solution of $Ay = b + e$ is

$$y = A^{-1}(b+e) = x + \frac{\delta_b}{\sigma_n}v_n$$

- relative change is

$$\frac{\|y-x\|}{\|x\|} = \frac{\sigma_1\delta_b}{\sigma_n} = \kappa(A)\,\delta_b$$

Nearest singular matrix

the singular matrix closest to A is

$$\sum_{i=1}^{n-1} \sigma_i u_i v_i^T = A + E \qquad \text{where } E = -\sigma_n u_n v_n^T$$

- this gives another interpretation of the condition number:

$$\|E\|_2 = \sigma_n = \frac{1}{\|A^{-1}\|_2}, \qquad \frac{\|E\|_2}{\|A\|_2} = \frac{\sigma_n}{\sigma_1} = \frac{1}{\kappa(A)}$$

  $1/\kappa(A)$ is the relative distance of A to the nearest singular matrix

- this also implies that a perturbation $A + E$ of A is certainly nonsingular if

$$\|E\|_2 < \frac{1}{\|A^{-1}\|_2} = \sigma_n$$

Bound on inverse

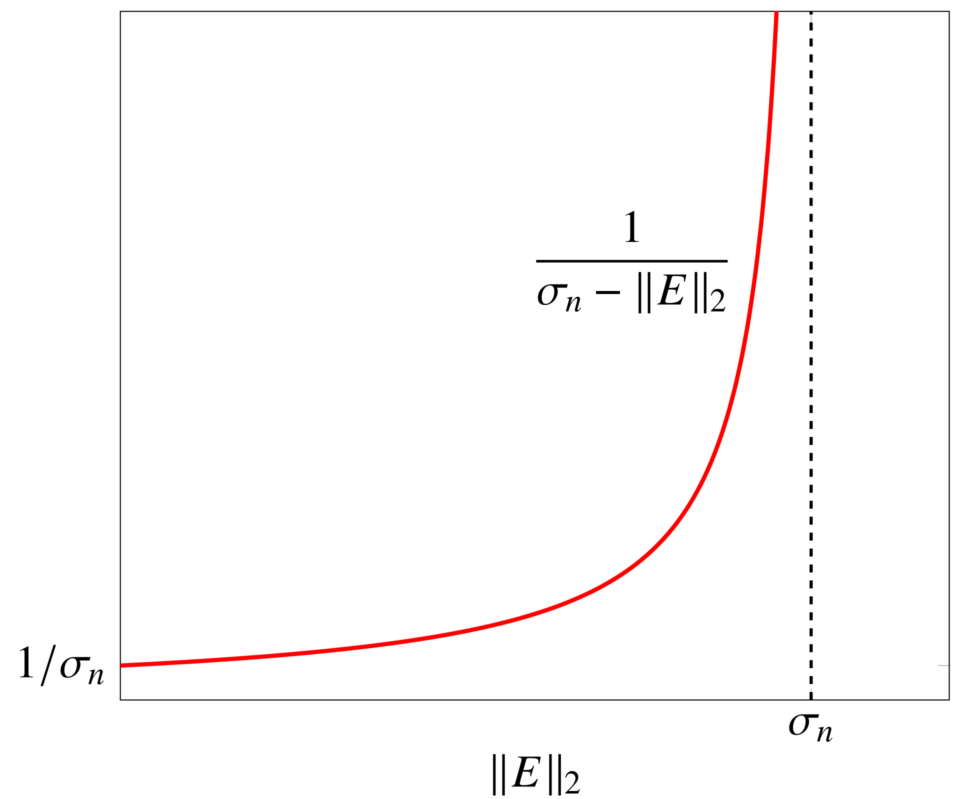
on the next page we prove the following inequality:

$$\|(A+E)^{-1}\|_2 \leq \frac{\|A^{-1}\|_2}{1 - \|A^{-1}\|_2 \|E\|_2} \qquad \text{if } \|E\|_2 < \frac{1}{\|A^{-1}\|_2} \tag{9}$$

using $\|A^{-1}\|_2 = 1/\sigma_n$:

$$\|(A+E)^{-1}\|_2 \leq \frac{1}{\sigma_n - \|E\|_2}$$

if $\|E\|_2 < \sigma_n$



Proof:

- the matrix $Y = (A+E)^{-1}$ satisfies

$$(I + A^{-1}E)Y = A^{-1}(A+E)Y = A^{-1}$$

- therefore

$$\begin{aligned} \|Y\|_2 &= \|A^{-1} - A^{-1}EY\|_2 \\ &\leq \|A^{-1}\|_2 + \|A^{-1}EY\|_2 \qquad \text{(triangle inequality)} \\ &\leq \|A^{-1}\|_2 + \|A^{-1}E\|_2\|Y\|_2 \end{aligned}$$

in the last step we use the property $\|CD\|_2 \leq \|C\|_2\|D\|_2$ of the matrix 2-norm

- rearranging the last inquality for $\|Y\|_2$ gives

$$\|Y\|_2 \leq \frac{\|A^{-1}\|_2}{1 - \|A^{-1}E\|_2} \leq \frac{\|A^{-1}\|_2}{1 - \|A^{-1}\|_2\|E\|_2}$$

in the second step we again use the property $\|A^{-1}E\|_2 \leq \|A^{-1}\|_2\|E\|_2$

Sensitivity to perturbations of coefficient matrix

linear equation with matrix A and perturbed matrix $A + E$:

$$Ax = b, \qquad (A + E)y = b$$

- we assume $\|E\|_2 < 1/\|A^{-1}\|_2$, which guarantees that $A + E$ is nonsingular
- bound on distance between the solutions:

$$\begin{aligned}
\|y - x\| &= \|(A+E)^{-1}(b - (A+E)x)\| \\
&= \|(A+E)^{-1}Ex\| \\
&\leq \|(A+E)^{-1}\|_2 \, \|E\|_2 \, \|x\| \\
&\leq \frac{\|A^{-1}\|_2\|E\|_2}{1 - \|A^{-1}\|_2\|E\|_2}\|x\| \qquad \text{(applying (9))}
\end{aligned}$$

- bound on relative change in solution in terms of $\delta_A = \|E\|_2/\|A\|_2$:

$$\frac{\|y - x\|}{\|x\|} \leq \frac{\kappa(A)\,\delta_A}{1 - \kappa(A)\delta_A} \tag{10}$$

Worst-case perturbation of coefficient matrix

an example where the upper bound (10) is sharp (from SVD $A = \sum_{i=1}^{n} \sigma_i u_i v_i^T$)

- choose $b = u_n$: the solution of $Ax = b$ is

$$x = A^{-1}b = (1/\sigma_n)v_n$$

- choose $E = -\delta_A \sigma_1 u_n v_n^T$ with $\delta_A < \sigma_n/\sigma_1 = 1/\kappa(A)$:

$$A + E = \sum_{i=1}^{n-1} \sigma_i u_i v_i^T + (\sigma_n - \delta_A \sigma_1) u_n v_n^T$$

- solution of $(A + E)y = b$ is

$$y = (A + E)^{-1} b = \frac{1}{\sigma_n - \delta_A \sigma_1} v_n$$

- relative change in solution is

$$\frac{\|y - x\|}{\|x\|} = \sigma_n \left(\frac{1}{\sigma_n - \delta_A \sigma_1} - \frac{1}{\sigma_n} \right) = \frac{\delta_A \kappa(A)}{1 - \delta_A \kappa(A)}$$

Exercises

Exercise 1

to evaluate the sensivity to changes in A, we can also look at the residual

$$\|(A+E)x-b\|$$

where $x = A^{-1}b$ is the solution of $Ax = b$

1. show that
$$\frac{\|(A+E)x-b\|}{\|b\|} \leq \kappa(A)\delta_A \qquad \text{where } \delta_A = \frac{\|E\|}{\|A\|}$$

2. show that for every A there exist b, E for which the inequality is sharp

Exercises

Exercise 2: consider perturbations in A and b

$$Ax = b, \qquad (A + E)y = b + e$$

assuming $\|E\|_2 < 1/\|A^{-1}\|_2$, show that

$$\frac{\|y - x\|}{\|x\|} \leq \frac{(\delta_A + \delta_b)\kappa(A)}{1 - \delta_A \kappa(A)}$$

where $\delta_b = \|e\|/\|b\|$ and $\delta_A = \|E\|_2/\|A\|_2$