

VI. SVD and principal components analysis

References:

[D] Demmel's book.

[S] Strang: Linear algebra and learning from data, Wellesley-Cambridge Press, 2019.

VI.1 Singular values and singular vectors [S, § I.8] [D, § 3.2.3]

Let $S \in \mathbb{R}^{n \times n}$ symmetric positive definite. Then

$$S = Q \Lambda Q^T$$

\uparrow orthogonal \nwarrow diagonal with positive entries

S has real and positive eigenvalues and orthogonal eigenvectors: the best we can hope!

The singular value decomposition (SVD) extends this factorization to any matrix, even outside the square case.

Let

A $m \times n$ -matrix ($m \geq n$)

There are two sets of singular vectors:

$u_1, \dots, u_m \in \mathbb{R}^m$
"left" singular vectors

$v_1, \dots, v_n \in \mathbb{R}^n$
"right" singular vectors

Both are orthogonal and are connected by

$$A v_i = \sigma_i u_i \quad i=1, \dots, n$$

$$\text{for } \sigma_1 \geq \dots \geq \sigma_n \geq 0$$

\nwarrow singular values

Set $r = \text{rank}(A)$. Then

u_1, \dots, u_r basis of $\text{Im}(A)$

v_{r+1}, \dots, v_n ————— $\text{Ker}(A)$

Matrix form:

$$U = (u_1 \dots u_m) \quad m \times m\text{-orthogonal}$$

$$V = (v_1 \dots v_n) \quad n \times n\text{-orthogonal}$$

Both U and V are square nonsingular and

$$U^{-1} = U^T$$

$$V^{-1} = V^T$$

$$\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r \\ \hline & & 0 \end{pmatrix} \begin{matrix} n \\ m-n \end{matrix} \quad m \times n$$

$\underbrace{\hspace{10em}}_n$

The (full) SVD is $A \cdot V = U \cdot \Sigma$ or equivalently

$$\boxed{A = U \cdot \Sigma \cdot V^T}$$

Example

$$\begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix} = \begin{pmatrix} 0.32 & -0.95 \\ 0.95 & 0.32 \end{pmatrix} \begin{pmatrix} 6.71 & 0 \\ 0 & 2.24 \end{pmatrix} \begin{pmatrix} 0.71 & 0.71 \\ -0.71 & 0.71 \end{pmatrix}$$

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

The column-row multiplication of $U \cdot \Sigma$ and V^T separates A into r pieces of rank 1:

$$A = \sigma_1 u_1 v_1^T + \dots + \sigma_r u_r v_r^T$$

In the example:

$$\begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix} = 6.71 \begin{pmatrix} 0.32 \\ 0.95 \end{pmatrix} \begin{pmatrix} 0.71 & 0.71 \end{pmatrix} + 2.24 \begin{pmatrix} -0.95 \\ 0.32 \end{pmatrix} \begin{pmatrix} -0.71 & 0.71 \end{pmatrix}$$
$$= \frac{3}{2} \begin{pmatrix} 1 & 1 \\ 3 & 3 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 3 & -3 \\ -1 & 1 \end{pmatrix}$$

The first piece is "more important" (or representative of A) because $\sigma_1 = 6.71 > \sigma_2 = 2.24$: this will be given a precise sense later.

The thin SVD avoids the 0's in the lower part of Σ and uses a diagonal matrix for the singular values:

$$A = U_n \cdot \Sigma_n \cdot V^T$$

with $U_n = (u_1, \dots, u_n)$ $n \times n$ -orthogonal

$\Sigma_n = \text{diag}(\sigma_1, \dots, \sigma_n)$ $n \times n$ -diagonal

The reduced SVD uses the nonzero singular values to remove the parts that are sure to produce zeros:

$$A = U_r \Sigma_r V_r^T$$

with $U_r = (u_1 \dots u_r)$ $m \times r$ -orthogonal

$\Sigma_r = \text{diag}(\sigma_1, \dots, \sigma_r)$ $r \times r$ -diagonal nonsingular

$V_r = (v_1 \dots v_r)$ $n \times r$ -orthogonal

We still have

$$U_r^T U_r = \mathbb{I}_r \quad V_r^T V_r = \mathbb{I}_r$$

but they are not invertible (since they are rectangular)

To identify the singular values and vectors we can consider the symmetric semipositive definite matrices

$$A^T A = (V \Sigma^T U^T) \cdot (U \Sigma V^T) = V \cdot \Sigma^T \Sigma \cdot V^T \quad n \times n$$

$$A \cdot A^T = (U \Sigma V^T) \cdot (V \Sigma^T U^T) = U \cdot \Sigma \Sigma^T U^T \quad m \times m$$

Then

V contains orthonormal eigenvectors of $A^T A$
 U contains orthonormal eigenvectors of $A A^T$

$\sigma_1, \dots, \sigma_r$ are the nonzero eigenvalues of both $A^T A$ and $A A^T$

To see the existence of the (full) SVD (and a way to compute it) we start with the diagonalization

$$A^T A = Q \Lambda Q^T$$

Let v_1, \dots, v_n be the columns of Q , ordered so that v_1, \dots, v_r correspond to the non-zero eigenvalues

$$\lambda_1 \geq \dots \geq \lambda_r \geq 0$$

$$\text{Set } \sigma_k = \lambda_k^{1/2} \quad k = 1, \dots, r$$

$$\text{Then } u_k = \sigma_k^{-1} A v_k \quad k = 1, \dots, r$$

~~gives~~ gives

$$A = (u_1 \dots u_r) \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_r \end{pmatrix} \begin{pmatrix} v_1^T \\ \vdots \\ v_r^T \end{pmatrix} \quad \text{reduced SVD}$$

because u_1, \dots, u_r are orthonormal: indeed

$$\langle u_j, u_k \rangle = u_j^T u_k = (\sigma_j^{-1} A v_j)^T (\sigma_k^{-1} A v_k) =$$

$$= \frac{1}{\sigma_j \sigma_k} v_j^T A^T A v_k = v_j^T v_k = \langle v_j, v_k \rangle \begin{cases} 1 & j=k \\ 0 & j \neq k \end{cases}$$

Exercise: show that u_1, \dots, u_r are eigenvalues of $A A^T$ with eigenvalues $\sigma_1^2, \dots, \sigma_r^2$.

To compute a full SVD, take ~~the~~

$$v_{r+1}, \dots, v_n \in \mathbb{R}^n \quad \text{and} \quad u_{r+1}, \dots, u_m \in \mathbb{R}^m$$

completing v_1, \dots, v_r and u_1, \dots, u_r to orthonormal basis. Then

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

$$\text{with } U = (u_1, \dots, u_m)$$

$$V = (v_1, \dots, v_n)$$

$$\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ 0 & & \sigma_r & & 0 \\ & & & & 0 \end{pmatrix}$$

Example: $A = \begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix}$

Then

$$A^T A = \begin{pmatrix} 25 & 20 \\ 20 & 25 \end{pmatrix} \quad \text{and} \quad A A^T = \begin{pmatrix} 9 & 12 \\ 12 & 41 \end{pmatrix}$$

The eigenvectors and eigenvalues of $A^T A$ are

$$\begin{pmatrix} 25 & 20 \\ 20 & 25 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 45 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 25 & 20 \\ 20 & 25 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = 5 \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

Right singular vectors

$$v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.71 \\ 0.71 \end{pmatrix}$$

$$v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -0.71 \\ 0.71 \end{pmatrix}$$

Singular values

$$\sigma_1 = \sqrt{45} = 6.71$$

$$\sigma_2 = \sqrt{5} = 2.24$$

Left singular values

$$u_1 = \sigma_1^{-1} A v_1 = \frac{1}{\sqrt{45}} \begin{pmatrix} 1 \\ 3 \end{pmatrix} = \begin{pmatrix} 0.32 \\ 0.95 \end{pmatrix} \quad u_2 = \sigma_2^{-1} A v_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} -3 \\ 1 \end{pmatrix} = \begin{pmatrix} -0.95 \\ 0.32 \end{pmatrix} \quad (6)$$

We conclude that $A = U \Sigma V^T$ with

$$U = \begin{pmatrix} 0.32 & -0.95 \\ 0.95 & 0.32 \end{pmatrix} \quad \Sigma = \begin{pmatrix} 6.71 & \\ & 2.24 \end{pmatrix} \quad V = \begin{pmatrix} 0.71 & -0.71 \\ 0.71 & 0.71 \end{pmatrix}$$

Some particular cases:

(1) Let S symmetric positive definite and

$$S = Q \Lambda Q^T$$

its diagonalization. Then $U = V = Q$ and $\Sigma = \Lambda$

(2) For an orthonormal $n \times n$ -matrix Q , all its singular values are equal to 1

(3) Let $A = x \cdot y^T$ be an $m \times n$ -matrix of rank 1 ($x \in \mathbb{R}^m$ and $y \in \mathbb{R}^n$). Its SVD (reduced) is

$$A = \underbrace{\frac{x}{\|x\|}}_{U_1} \cdot (\|x\| \cdot \|y\|) \underbrace{\frac{y^T}{\|y\|}}_{V_1^T}$$

Σ_1

The geometry of the SVD:

The SVD separates the matrix into
orthogonal \times diagonal \times orthogonal

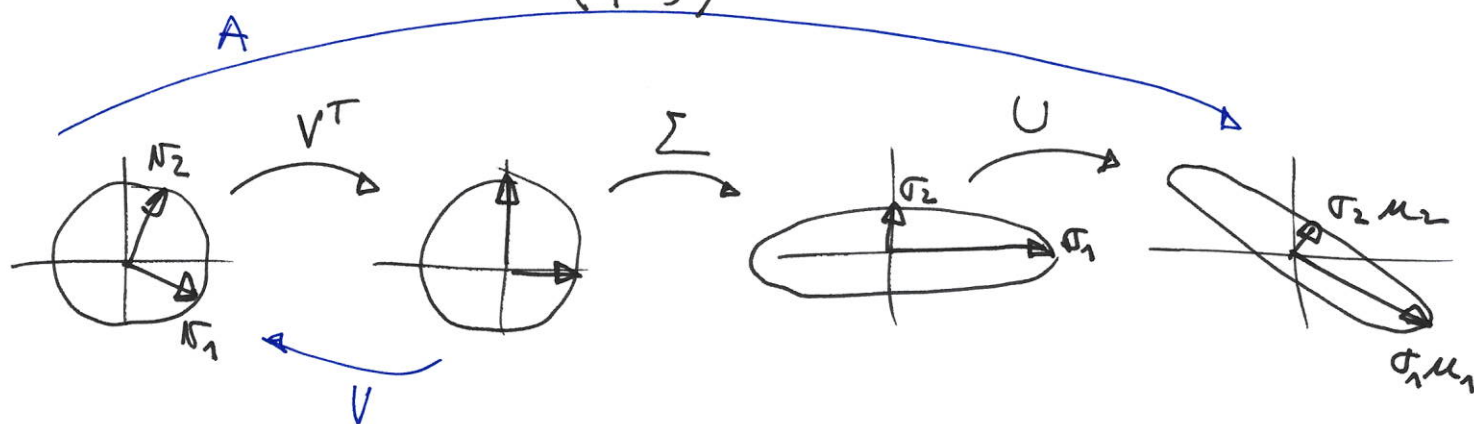
The unit sphere \mathbb{S}_n of \mathbb{R}^n is sent to an
ellipsoid $A\mathbb{S}_n$ of \mathbb{R}^n centered at the
origin and with axes

$$\sigma_i u_i \quad i=1, \dots, r$$

~~##~~ In two dimensions, we can draw the process.

Example

$$A = \begin{pmatrix} 3 & 0 \\ 4 & 5 \end{pmatrix}$$



VI.2 The best low rank approximation

[D, §3.2.3], [S, §I.9]

The 2-norm can be computed in terms of the SVD

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

We have $\|A\|_2 = \sigma_1$

Indeed, the 2-norm is invariant under multiplication by orthogonal matrices and so

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

The Frobenius norm is also invariant under multiplication by orthogonal matrices and so

$$\|A\|_F = \|U^T \cdot A \cdot V\|_F = \|\Sigma\|_F = (\sigma_1^2 + \dots + \sigma_r^2)^{1/2}$$

$$(\sum_{i,j} a_{ij}^2)^{1/2}$$

The Eckart-Young theorem says that for $k = 1, \dots, r$ the matrix

$$A_k = \sigma_1 u_1 v_1^T + \dots + \sigma_k u_k v_k^T = U_k \cdot \Sigma_k \cdot V_k^T$$

is the best rank k approximation of A in ~~either~~ both the 2-norm and the Frobenius norm.

Indeed for both norms

$$\|A - A_k\| = \|\Sigma - \Sigma_k\| = \left\| \begin{pmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \\ & & & 0 & \dots & 0 \end{pmatrix} \right\|$$

orthogonal invariance

and so

$$\|A - A_k\|_2 = \sigma_{k+1}$$

$$\|A - A_k\|_F = (\sigma_{k+1}^2 + \dots + \sigma_r^2)^{1/2}$$

The theorem says that for both norms

$$\|A - B\| \geq \|A - A_k\|$$

for any other k -rank $m \times n$ -matrix B .

An application: image compression.

A B/W image of $m \times n$ pixels can be coded by an $m \times n$ -matrix A with entries $0 \leq a_{ij} \leq 1$

(the brightness of the pixel (i,j))

black white
0 gray 1
~~white~~

The size of the image is mn

Instead of storing/transmitting it, we can replace it by the k -rank approximation

$$A_k = \sum_{i=1}^k \sigma_i u_i v_i^T$$

(or $k(m+n)$ storing u_i, v_i)

of size $k \cdot (1+m+n)$

The relative error of the approximation is

$$\frac{\|A - A_k\|_2}{\|A\|_2} = \frac{\sigma_{k+1}}{\sigma_1}$$

and the compression ratio is

$$\frac{p_k(m+n)}{m \cdot n}$$

A 320×200 photo of a clown and its approximations

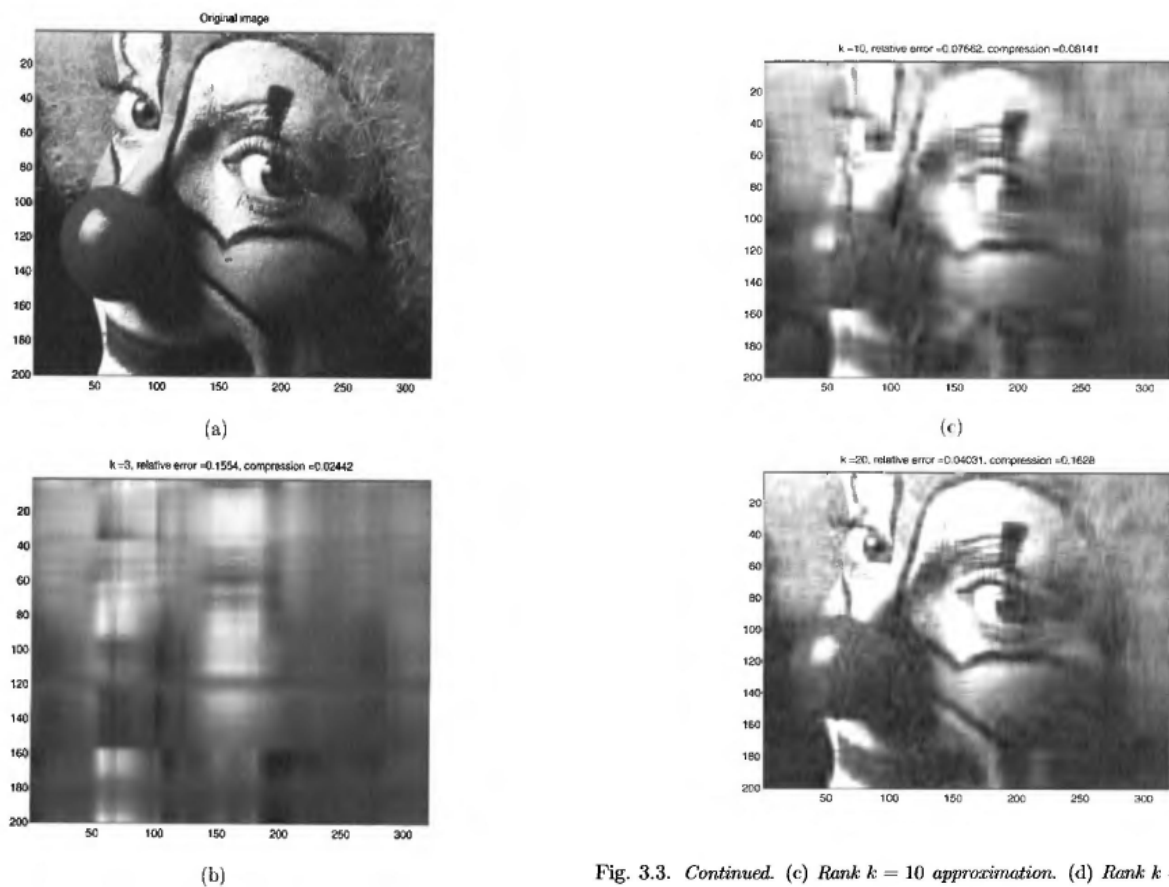


Fig. 3.3. Image compression using the SVD. (a) Original image. (b) Rank $k=3$ approximation.

Fig. 3.3. Continued. (c) Rank $k=10$ approximation. (d) Rank $k=20$ approximation.


VI.6 Principal components analysis

[S, ±.9], [Schlens]

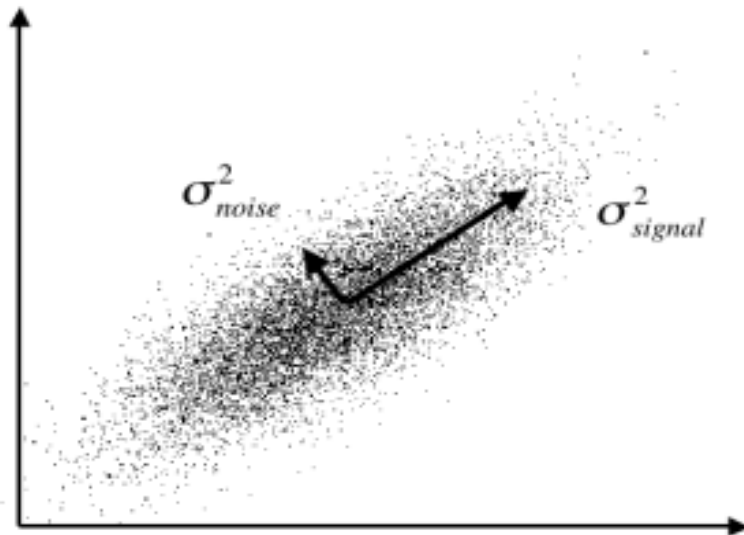
[S] Strang's book

[Schlens] Schlens, A tutorial on PCA, 2003.

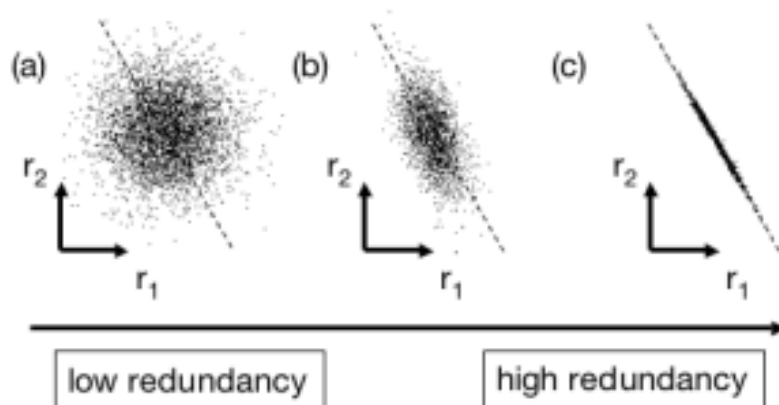
Let M be an $m \times n$ data matrix: the rows are samples and the columns are variables, like in

$M =$  $m \times 2$ matrix

Can we simplify the description of this data?
Plotting the samples in \mathbb{R}^2 and centering them,
they might correlated:



This correlation might be higher or lower
 more [↑] ~~significant~~ [↑] less ~~significant~~



The key parameters in probability and statistics:

mean

variance

The mean is

$$\mu = \frac{1}{m} \sum_{i=1}^m M_i \in \mathbb{R}^n$$

The centered data is

$$A = M - \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \mu^T = \begin{pmatrix} M_1 - \mu^T \\ \vdots \\ M_m - \mu^T \end{pmatrix} = \begin{pmatrix} A_1 \\ \vdots \\ A_m \end{pmatrix}$$

The mean of each variable in A is 0.

[↑]
column

The variances and covariances of $A = (a_1 \dots a_n)$ are the diagonal and off-diagonal entries of

$$A^T A$$

The covariance matrix is

$$S = \frac{1}{n-1} A^T \cdot A$$

\uparrow $n-1$ degrees of freedom

$n \times n$ symmetric
semipositive definite

Example

$$A = \begin{pmatrix} 3 & 7 \\ -4 & -6 \\ 7 & 8 \\ 1 & -1 \\ -4 & -1 \\ -3 & -7 \end{pmatrix}$$

centered data matrix
of ages and heights

Then

$$S = \frac{1}{6-1} A^T A = \begin{pmatrix} 20 & 25 \\ 25 & 40 \end{pmatrix} \quad \text{covariance matrix}$$

Let

$$A = U \cdot \Sigma \cdot V^T \quad \text{thin SVD}$$

and set

$$B = A \cdot V = U \Sigma \quad m \times n$$

Then

$$\frac{1}{n-1} B^T B = \frac{1}{n-1} \Sigma^2 \quad \text{diagonal}$$

the variables in B are not correlated
and ordered by their variance $\langle b_i, b_i \rangle = \sigma_i^2 \quad \langle b_i, b_j \rangle = 0 \quad i \neq j$

The matrix

$$V = (v_1 \dots v_n)$$

gives an orthonormal basis of \mathbb{R}^n .

The representation of a vector $x \in \mathbb{R}^n$ wr. to this basis is

$$x = \sum_{j=1}^n \langle x, v_j \rangle v_j$$

Hence

$$B = A \cdot V = \left(\langle A_i, v_j \rangle \right)_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}}$$

components of A_i
w.r. to the basis v_1, \dots, v_n

For $1 \leq k \leq n$ the first k columns of B

$$b_1, \dots, b_k \in \mathbb{R}^m$$

are uncorrelated and have total variance

$$\frac{1}{m-1} (\sigma_1^2 + \dots + \sigma_k^2)$$

~~This is the result~~ These columns give the projection of the samples in A to the linear subspace

$$\text{Vect}(v_1, \dots, v_k)$$

The projected data has maximal total variance (among all possible orthogonal projections of the data to a k -linear subspace of \mathbb{R}^n)

Also the sum of the squares of the distances between the samples and its projections is minimized for this k -linear subspace:

$$\sum_{i=1}^m \|A_i - \sum_{j=1}^k \langle A_i, N_j \rangle N_j\|_2^2 = \sum_{i=1}^m \sum_{j=k+1}^n \langle A_i, N_j \rangle^2 = \|A - A_k\|_F^2$$

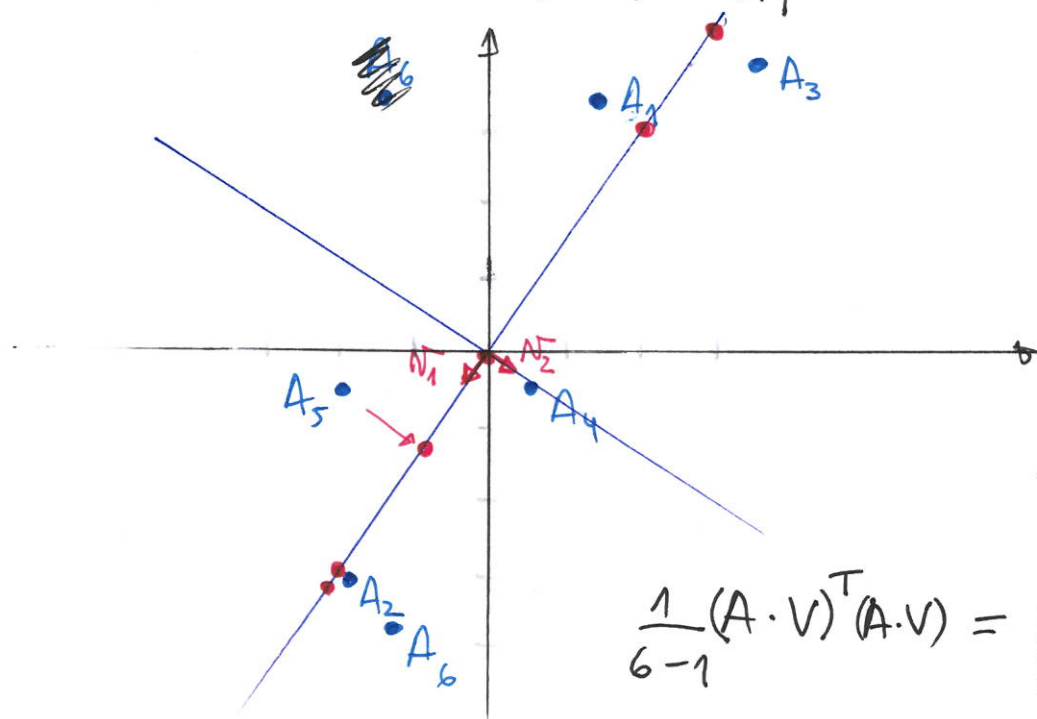
best k -rank approximation

Frobenius norm

This is a consequence of the Eckart-Young theorem

Example (cont)

$$A = \begin{pmatrix} 3 & 7 \\ -4 & -6 \\ 7 & 8 \\ 1 & -1 \\ -4 & -1 \\ -3 & -7 \end{pmatrix} = U \cdot \Sigma \cdot V^T = \begin{pmatrix} -0.44 & -0.36 \\ 0.43 & 0.01 \\ -0.63 & 0.33 \\ 0.02 & 0.35 \\ 0.18 & -0.70 \\ 0.44 & 0.37 \end{pmatrix} \cdot \begin{pmatrix} 16.87 & 0 \\ 0 & 3.92 \end{pmatrix} \cdot \begin{pmatrix} -0.56 & -0.83 \\ +0.83 & -0.56 \end{pmatrix}$$



1st variance

$$\frac{1}{6-1} (A \cdot V)^T (A \cdot V) = \begin{pmatrix} 56.92 & 0 \\ 0 & 3.07 \end{pmatrix}$$

2nd variance (16)

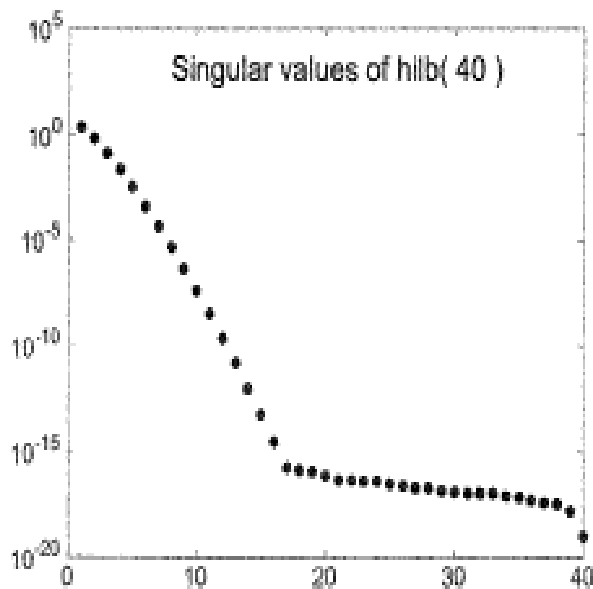
The principal components

$$b_i = \sigma_i u_i \quad i=1, \dots, k$$

account for

$$\rho_k = \frac{\sum_{i=1}^k \sigma_i^2}{\sum_{i=1}^n \sigma_i^2}$$

of the total variance of the data. The choice of k should keep the true signal and discard the noise



$$H_{ij} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{3} & \cdot & \cdot \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \cdot & \cdot \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} = \frac{1}{(i+j-1)}$$

Figure I.12: Scree plot of $\sigma_1, \dots, \sigma_{39}$ ($\sigma_{40} = 0$) for the evil Hilbert matrix, with elbow at the effective rank: $r \approx 17$ and $\sigma_r \approx 10^{-16}$.

VI.4 The rank deficient LSP revisited [D, §3.5]

The SVD applies also to the LSP, and it is particularly appropriate for the rank deficient case.

Let

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

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

If $r < n$ then the solution of the LSP

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2$$

is not unique since

$$A\hat{x} = A(\hat{x} + y)$$

$$\forall y \in \text{Ker}(A) \cong \mathbb{R}^{n-r}$$

A reasonable choice is the minimizer with the smallest norm

Let

$$\begin{array}{ccc} \begin{array}{c} m \\ \boxed{A} \\ n \end{array} = \begin{array}{c} m \\ \boxed{U} \\ m \end{array} \begin{array}{c} \boxed{\Sigma} \\ n \end{array} \begin{array}{c} \boxed{V^T} \\ n \end{array} = \begin{array}{c} m \\ \boxed{U_r} \\ r \end{array} \begin{array}{c} r \\ \boxed{\Sigma_r} \\ r \end{array} \begin{array}{c} \boxed{V_r^T} \\ n \end{array} \\ \text{Full SVD} & & \text{reduced SVD} \end{array}$$

$$U = (u_1 \dots u_m)$$

$$\Rightarrow$$

$$U_r = (u_1 \dots u_r)$$

$$V = (v_1 \dots v_n)$$

$$\Rightarrow$$

$$V_r = (v_1 \dots v_r)$$

$$\Sigma = \begin{pmatrix} \sigma_1 & & 0 \\ & \ddots & \\ & & \sigma_n \\ 0 & & \end{pmatrix}$$

$$\Rightarrow$$

$$\Sigma_r = \text{diag}(\sigma_1, \dots, \sigma_r)$$

The Moore-Penrose inverse of A is

$$A^+ = V_r \Sigma_r^{-1} U_r^T \quad n \times m \text{-matrix}$$

The solution of the LSP is

$$\boxed{\hat{x} = A^+ b}$$

When A is rank deficient (i.e. $r < n$) it is the solution with the smallest norm.

It is well conditioned if the smallest non zero singular value of A is not too small.

changing b to $b + \delta b$ changes x to $x + \delta x$ with

$$\boxed{\|\delta x\|_2 \leq \frac{\|\delta b\|_2}{\sigma_r}}$$

because

$$\delta x = V_r \Sigma_r^{-1} U_r^T \delta b$$

$$\text{and so } \|\delta x\|_2 \leq \|\Sigma_r^{-1}\|_2 \|\delta b\|_2 = \frac{\|\delta b\|_2}{\sigma_r}$$

In practice, the difficulty is that the rank is not continuous, and so affected by small perturbations

Example

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

$$b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Then

$$A^+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \cdot (1) \cdot (1 \ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\hat{x} = A^+ b = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

with condition number $\frac{1}{\sigma_1} = 1$

Let $\varepsilon > 0$ and

$$A_\varepsilon = \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}$$

gives

$$\hat{x}_\varepsilon = \begin{pmatrix} 1 \\ 1/\varepsilon \end{pmatrix}$$

Hence round off will make perturbations of size $O(\varepsilon) \|A\|_2$, that might increase the condition number from $1/\sigma_1$ to $1/\varepsilon$.

The SVD is backward stable: round-off with machine epsilon ε gives

$$(U + \delta U)(\Sigma + \delta \Sigma)(V + \delta V)^T = A + \delta A$$

with

$$\|\delta A\|_2 \leq O(\varepsilon) \|A\|_2$$

Hence the computed singular values $\sigma_i + \delta \sigma_i$ verify

$$|\delta \sigma_i| \leq O(\varepsilon) \|A\|_2$$

Let $\boxed{\text{tol} > 0}$ be a user supplied measure
of uncertainty in A .

Round off implies

$$\text{tol} \geq \varepsilon \|A\|_2$$

$\nwarrow \sigma_1$

but it might be larger (eg. errors in measurements)

Given

$\tilde{U}, \tilde{\Sigma}, \tilde{V}$ computed SVD of A

set
$$\hat{\sigma}_i = \begin{cases} \tilde{\sigma}_i & \text{if } \tilde{\sigma}_i \geq \text{tol} \\ 0 & \text{else} \end{cases}$$

and replace $\tilde{\Sigma}$ by

$$\hat{\Sigma} = \begin{pmatrix} \tilde{\sigma}_1 & \dots & \tilde{\sigma}_r & 0 & \dots & 0 \\ & & & & & \\ & & 0 & & & \end{pmatrix} \quad \text{truncated SVD}$$

and

$$\hat{X} = \tilde{V}_r \hat{\Sigma}_r^{-1} \tilde{U}_r^T$$

The error is bounded by $\delta(\text{tol})$ and the
condition number by $1/\sigma_r$.