ENGSCI 721

INVERSE PROBLEMS

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MODULE OVERVIEW

Inverse Problems (*Oliver Maclaren*) [~8 lectures/2 tutorials]

1. *Basic concepts* [4 lectures]
   Forward vs inverse problems. Well-posed vs ill-posed problems. Algebra and calculus of inverse problems (matrix calculus, generalised inverses etc). Regularisation and trade-offs.
2. *More regularisation* [3 lectures]
   Higher-order Tikhonov regularisation, truncated singular value decompositions, iterative regularisation.

MODULE OVERVIEW

3. *Preview of the statistical view of inverse problems* [1 lectures]
   Bayesians, Frequentists and all that. Basic frequentist analysis.

LECTURE 6: REGULARISATION IN LINEAR PROBLEMS: SVD AND TSVD

Topics:

- Singular Value Decomposition
  - The ‘crown jewel’ of linear algebra!
  - Generalises eigenvalue analysis to general (non-square etc) matrices
- Truncated Singular Value Decomposition
  - As regularisation scheme
  - Relation to Tikhonov regularisation

EngSci 721 : Lecture 6

Regularisation in linear problems :
The Singular Value Decomposition perspective

- SVD (type of matrix factorisation)
  - └ extension of eigen analysis
  - └ insight/calculation for inverses, resolution, effect of regulars.
  - └ the 'crown jewel' of linear algebra
- Truncated SVD.
  - └ as regularisation scheme.
  - └ connection to Tikhonov.

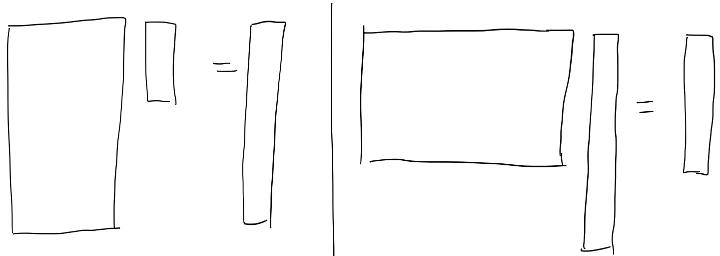
__Bonus__ : rank factorisation & extension to nonlinear epi-mono factorisations

Eigenvalues

Recall that for a square matrix A, eigenvalues solve

$$\boxed{Ax = \lambda x}$$

However, we are interested in <u>non-square</u> matrices in inverse problems (& statistics etc)!



Tall/overdetermined systems
- 'classical statistics'

Wide/underdetermined systems
- 'inverse problems'
- 'nonparametric statistics'
- 'machine learning' etc

→ eigenvalues don't make sense for non-square!

Eigenvalues?

A $m \times n$

x n

y m

$Ax = y$

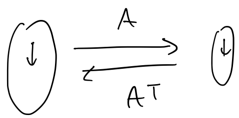
$\underbrace{Ax}_{\in \mathbb{R}^m} = \underbrace{\lambda x}_{\in \mathbb{R}^n}$ doesn't make sense

} live in different spaces!

Solutions?

related {

- Consider different bases for each space
- Consider eigenvalues of square matrices like A^TA & AA^T:



A^TA: $\mathbb{R}^n \to \mathbb{R}^n$

AA^T: $\mathbb{R}^m \to \mathbb{R}^m$

Singular values & singular vectors I.

Instead of $Av = \lambda v$ } eigenvector v, eigenvalue λ

we consider $\boxed{Av = u\sigma}$

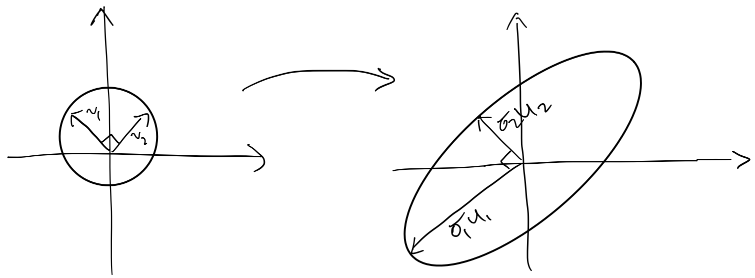
matrix, vector, vector, scalar

Solutions: $\{(u_i, \sigma_i, v_i)\}$

left singular vector (data space)

singular value

right singular vector (model space)



model space $\mathbb{R}^n$

x

data space $\mathbb{R}^m$

y

Singular values & singular vectors II

In particular, for singular vectors / values

$$\boxed{A v_i = u_i \sigma_i}$$

we require $\{v_i\}$ & $\{u_i\}$ to both be

$\boxed{\text{orthonormal}}$ $\left\{ \begin{array}{l} \text{orthogonal} \\ \text{unit length} \end{array} \right\} \Rightarrow$ LI

sets of vectors.

eg $\quad u_i^T u_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$ etc

& that they $\boxed{\text{span}}$ their respective spaces

while $\boxed{\sigma_i \geq 0}$ are non-negative.

In contrast to eigenvalues/vectors, we can always work with singular values/vectors

→ generalisation to nonsquare matrices

Singular value decomposition (SVD) I.

Suppose for the moment all rows are independent & consider all $\boxed{A v_i = u_i \sigma_i}$ sol^{n}s ($\sigma_i \geq 0$):

$$\underset{m \times n}{m \overset{n}{\begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix}}} \underset{n \times n}{\overset{n}{\begin{bmatrix} \vdots & \vdots & & \vdots \\ v_1 & v_2 & \cdots & v_n \\ \vdots & \vdots & & \vdots \end{bmatrix}}} = \underset{m \times m}{\overset{m}{\begin{bmatrix} \vdots & \vdots & & \vdots \\ u_1 & u_2 & \cdots & u_m \\ \vdots & \vdots & & \vdots \end{bmatrix}}} \underset{m \times n}{\begin{bmatrix} \sigma_1 & & & 0 & \cdots & 0 \\ & \ddots & & \vdots & & \vdots \\ & & \sigma_m & 0 & \cdots & 0 \end{bmatrix}}$$

where $\{v_i\}$ & $\{u_i\}$ are orthonormal sets

ie $\quad \boxed{AV = U\Sigma}$, V & U are orthogonal matrices, V $n \times n$, U $m \times m$

Note: n cols of A not LI, but n v vectors are (why?)

$\Rightarrow$ V & U are invertible, with inverses $V^{-1} = V^T$, $U^{-1} = U^T$

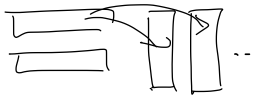
→

Side note: matrix multiplication [see eg Golub & van Loan]

$\boxed{\text{AB can be thought of in multiple ways}}$

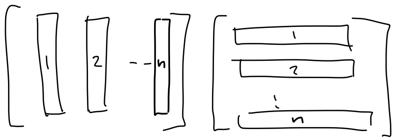
Here:
$A_{m\times n}$, $B_{n\times p}$
$A[:,i]$ = ith col of A
$A[i,:]$ = ith row of A
etc.

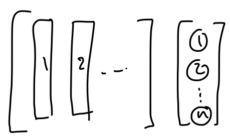
1. → usual $\boxed{\text{'rows of A times cols of B'}}$ (inner product entries)

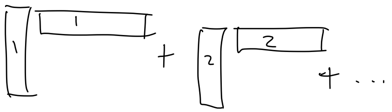


$$\cdots = \begin{bmatrix} A[1,:]B[:,1] & \cdots & A[1,:]B[:,p] \\ \vdots & & \\ A[m,:]B[:,1] & \cdots & A[m,:]B[:,p] \end{bmatrix}$$ ('dot product form')

2. → generalised version of linear combo of A's cols from matrix times vector rule:



(cf: )



ie $\boxed{\text{'sum of outer products'}}$:

$$\boxed{AB = \sum_i A[:,i]B[i,:]}$$

$\left(= \sum a_i b_i^T\right.$ if $A = \begin{bmatrix} a_1 & a_2 & \cdots \end{bmatrix}$ (col. partition) & $B = \begin{bmatrix} b_1^T \\ b_2^T \\ \vdots \end{bmatrix}$ $\left.\right)$ (row partition)

Note: common notation $b_1^T = B[1,:]$

"Transpose of col. partition of B^T", not transp. of col part. of B!

3. → matrix A times each col of B

ie $\boxed{\text{'multiple RHS'}}$ form

$$A\begin{bmatrix} \boxed{1} & \boxed{2} & \cdots & \boxed{\ } \end{bmatrix} = \begin{bmatrix} A\boxed{1} & A\boxed{2} & \cdots & A\boxed{p} \end{bmatrix}$$

$$= \left[\, AB[:,1] \;\vdots\; AB[:,2] \;\vdots\; \cdots \;\vdots\; AB[:,p] \,\right]$$

Exercise:

verify $Av_i = u_i\sigma_i$ can be written $AV = U\Sigma$ as given on prev. page, when rank $= m$, $n > n$, by considering

$$\begin{array}{c c} & n \\ m & \begin{bmatrix} & & \\ & A & \\ & & \end{bmatrix} \end{array} \begin{array}{c} n \\ \begin{bmatrix} \vdots & \vdots & & \\ v_1 & v_2 & \cdots & v_n \\ \vdots & \vdots & & \end{bmatrix} \end{array} n$$

$$\begin{array}{c c} & m \\ m & \begin{bmatrix} \vdots & & \vdots \\ u_1 & \cdots & u_m \\ \vdots & & \vdots \end{bmatrix} \end{array} \begin{array}{c c} & \begin{array}{cc} m & n-m \end{array} \\ m & \left[\begin{array}{ccc|c} \sigma_1 & & 0 & \\ & \ddots & & 0 \\ 0 & & \sigma_m & \end{array}\right] \end{array}$$

[Note: there may be multiple $\sigma = 0$ sol^{n}s!]

Exercise:

verify $AB^T = \sum_i a_i b_i^T$, for col partitions:

$$A = \begin{bmatrix} a_1 & a_2 & \cdots \end{bmatrix},\; B = \begin{bmatrix} b_1 & b_2 & \cdots \end{bmatrix}$$

(note: B not B^T!)

Singular value decomposition (SVD) II.

The SVD is then given by:

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

Every matrix has an SVD

$\rightarrow$ if A is $m \times n$ with rank r

then U & V still $m \times m$ & $n \times n$ (span $\mathbb{R}^m$ & $\mathbb{R}^n$), while

$$\Sigma = \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix}$$ block matrix shape $m \times n$

& Σ_r is $r \times r$ diagonal matrix with positive entries, & ordered as $\sigma_1 \geq \sigma_2 \geq \dots \sigma_r \geq 0$

Compact/reduced form: (rank r)

$$\boxed{A = U_r \Sigma_r V_r^T}$$

U_r: first r col of U
V_r: first r col of V

ie $A = [U_r, U_0] \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} [V_r, V_0]^T$

Some Properties of SVD

- if a matrix has rank r then it has r non-zero singular values $\Big\}$ (as hinted prev. pages)

- $A = U \Sigma V^T = U_r \Sigma_r V_r^T$

- $A^T = V \Sigma^T U^T = V_r \Sigma_r U_r^T$ $\Big\}$ $A^T U = V \Sigma^T$ U basis for data, V for model space.

- $A^T A = V \Sigma^T U^T U \Sigma V^T$
  $= V \Sigma^2 V^T$
  $= V_r \Sigma_r^2 V_r^T$

- $A A^T = U \Sigma V^T V \Sigma^T U^T$
  $= U \Sigma \Sigma^T U^T$
  $= U_r \Sigma_r^2 U_r^T$

Eigen for model/data

$$\mathbb{R}^n \underset{A^T}{\overset{A}{\rightleftarrows}} \mathbb{R}^m$$

$A^T A$ $n \times n$ $A A^T$

V $n \times n$ basis v_i U $m \times m$ basis u_i

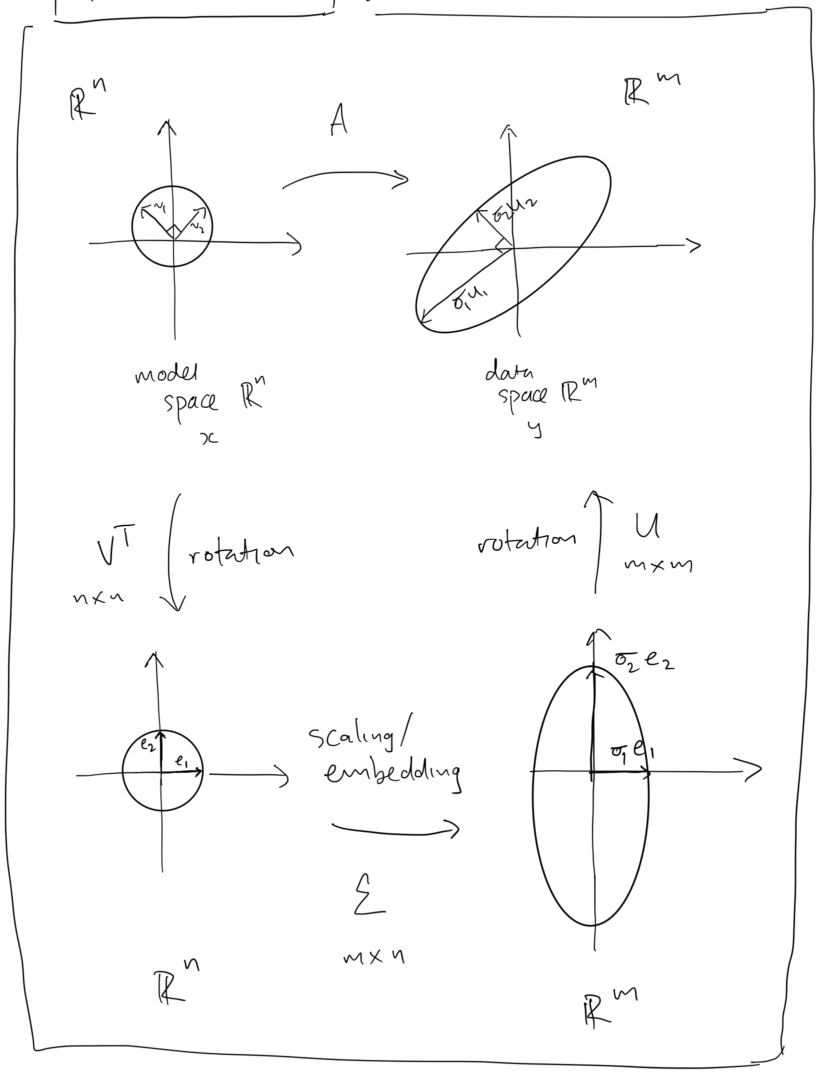
$\rightarrow$ σ_i^2 are the non-zero eigenvalues of $A^T A$ & of $A A^T$

$\rightarrow$ associated (non-zero σ_i) u_i & v_i are eigenvectors of $A A^T$ & $A^T A$ respectively

---

SVD : interpretation

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



SVD : Big picture

Key advantage : $\boxed{\text{explicit calculation}}$

- inverses (left, right, pseudo)
- model/data resolution operators
- stability/instability depending on singular values
- stablised approximations via truncation
- effect of Tikhonov (etc) regularisation on singular values

Disadvantage : though some intutions transfer to nonlinear, essentially a linear concept.

(But see <u>rank factorisation</u>)

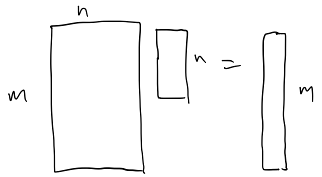
SVD & Inverses (Left / Retraction)

Recall:

A left inverse satisfies $\boxed{LA = I}$ $\left.\right\}$ A $m \times n$, L $n \times m$, I $n \times n$

&

a left inverse exists when # rows $\geq$ # cols of A & the cols are LI



U $m \times m$

V $n \times n$

Given $\boxed{A = U_n \Sigma_n V_n^T}$, $\boxed{\text{rank} = n}$

Consider:

$$\boxed{L = \underbrace{\underbrace{V_n}_{n \times n} \underbrace{\Sigma_n^{-1}}_{n \times n} \underbrace{U_n^T}_{n \times m}}_{n \times m}} \quad , \quad \Sigma_n^{-1} = \begin{bmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_n} \end{bmatrix}$$

$$LA = V_n \Sigma_n^{-1} U_n^T U_n \Sigma_n V_n^T$$

$$= I \qquad (n \times n)$$

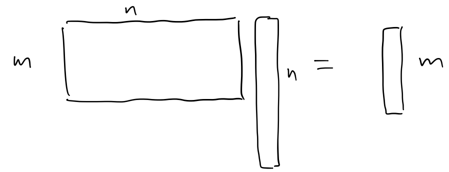
SVD & Inverses (Right / Section)

Recall:

A right inverse satisfies $\boxed{AR = I}$ $\left.\right\}$ A $m \times n$, R $n \times m$, I $m \times m$

&

a right inverse exists when # cols $\geq$ # rows of A & the rows are LI



U $m \times m$

V $n \times n$

Given $\boxed{A = U_m \Sigma_m V_m^T}$, $\boxed{\text{rank} = m}$

Consider:

$$\boxed{R = \underbrace{\underbrace{V_m}_{n \times m} \underbrace{\Sigma_m^{-1}}_{m \times m} \underbrace{U_m^T}_{m \times m}}_{n \times m}} \quad , \quad \Sigma_m^{-1} = \begin{bmatrix} \frac{1}{\sigma_1} & & \\ & \ddots & \\ & & \frac{1}{\sigma_m} \end{bmatrix}$$

$$AR = U_m \Sigma_m V_m^T V_m \Sigma_m^{-1} U_m^T$$

$$= I \qquad (m \times m)$$

SVD & The Generalised (Pseudo) inverse

In general, given

$$\boxed{A = U_r \Sigma_r V_r^T}, \quad \boxed{\text{rank } r}$$

we have the generalised (pseudo) inverse:

$$\boxed{A^\dagger = V_r \Sigma_r^{-1} U_r^T}$$

explicit formula ... & ... recall V, U, σ related to A^TA & AA^T eigen.

→ The generalised inverse is usually computed via SVD

→ We have seen that the generalised inverse needs regularisation

↳ New idea: truncate SVD for $p < r$

But first ..... recall

Model resolution, data resolution operators:

$\boxed{R_D = AA^\dagger}$ } how much data is 'shrunk' or smeared

$\boxed{R_M = A^\dagger A}$ } how much model is 'shrunk' or smeared

see below

Not I in gen. but something 'similar'

→ Note $I^2 = I$ ('idempotent')

Projection operators P characterised by

$\boxed{P^2 = P}$ ('idempotent')

→ one application of P gives 'maximum' effect

1. Suppose $A^\dagger A = I$ but $AA^\dagger \neq I$ (left inverse only)

$$\Rightarrow R_D R_D = AA^\dagger AA^\dagger = AA^\dagger = R_D$$

$\Rightarrow R_D$ is a projection on data space

2. Suppose $AA^\dagger = I$ but $A^\dagger A \neq I$ (right inverse only)

$$R_M R_M = A^\dagger A A^\dagger A = A^\dagger A = R_M$$

$\Rightarrow R_M$ is a projection on model space.

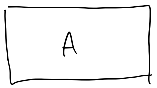
SVD & Resolution : Explicit calculation.

Now : $\boxed{R_D = U_r U_r^T}$ $m \times m$ $\begin{cases} U_r & m \times r \\ U_r^T & r \times m \end{cases}$ (r $m$vectors)

$\boxed{R_M = V_r V_r^T}$ $n \times n$ $\begin{cases} V_r & n \times r \\ V_r^T & r \times n \end{cases}$ (r $n$vectors)

- If rank $r = m < n$

$\Rightarrow R_D = I_m$



(recover data exactly)
(models are 'reduced')

But $R_M \neq I_n$

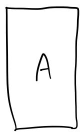
Though $R_M^2 = V_r \underline{V_r^T V_r} V_r^T = V_r V_r^T = R_M$

$\Rightarrow$ R_M is model projection operator

- If rank $r = n < m$

$R_D \neq I_m$

$R_M = I_n$



(data are 'reduced')
(models recovered exactly.)

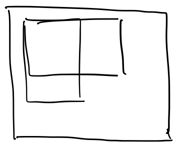
though $R_D = U_r \underline{U_r^T U_r} U_r^T = U_r U_r^T = R_D$

$\Rightarrow$ R_D is data projection

- If rank $r < m$ & n

$R_D \neq I_m$

$R_M \neq I_n$



$\Rightarrow$ Both are projection operators.
($U_r^T U_r = I$, $V_r^T V_r = I$ still)

Exercise (Tut/Assignments) :

Explore model/data resolution operators for typical inverse problem examples seen so far

$\longrightarrow$

So.... regularisation!

→ singular values may be positive but effectively zero (machine tol. etc)

⇒ cause: $\boxed{\text{effective rank } p < \text{rank } r}$

→ small singular values cause instability

Key: inverse leads to $\boxed{\text{dividing by small } \sigma_i \text{ values}}$

SVD as basis expansion:

$$A^{\dagger} = V_r \Sigma_r^{-1} U_r^T = \sum_i^r \left(v_i \frac{1}{\sigma_i} u_i^T \right)$$

& $x^{\dagger} = A^{\dagger} y$

$$= \sum_i^r \left(v_i \frac{1}{\sigma_i} u_i^T y \right)$$

$$= \mathrm{Sum}\left[\underbrace{\left(\frac{u_i^T y}{\sigma_i} \right)}_{\text{coeff.}} \underbrace{v_i}_{\text{basis vector in model space}} \right]$$

coeff.: Large for $\sigma_i \to 0$

Stability

consider $x^{\dagger} = A^{\dagger} y$

& $x^{\dagger\prime} = A^{\dagger} y'$

for small data perturbation

$$\| y - y' \|_2 < \delta$$

Then $x^{\dagger} - x^{\dagger\prime} = A^{\dagger}(y - y')$

& $\| x^{\dagger} - x^{\dagger\prime} \|_2 \leq \| A^{\dagger} \|_2 \| y - y' \|_2$

$$\boxed{\text{where } \| A \|_2 := \max_{\|x\|_2 = 1} \| A x \|_2 = \sigma_1 = \text{largest singular value}}$$

Leads to (with other details...)

$$\boxed{\frac{\| x^{\dagger} - x^{\dagger\prime} \|_2}{\| x^{\dagger} \|_2} \leq \frac{\sigma_1}{\sigma_r} \frac{\| y - y' \|_2}{\| y \|_2}}$$

σ_1: largest singular value

σ_r: smallest singular value.

Stability : Key point

Stability (continuity modulus) of A^+ governed by

$$\boxed{\mathrm{cond}(A^+) = \frac{\sigma_1}{\sigma_r}}$$

(condition number)

Key trade-off :

truncate singular value expansion

↳ more stable (less 'variance')

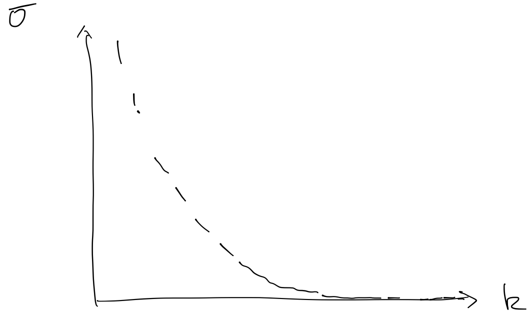
↳ biased (model resolution less like identity

→ favour particular models)

(stats : Bias-Variance tradeoff)

Spectrum

Plot of singular values in decreasing order :



Key : $\boxed{\text{Ill-posed}}$

→ no clear gap

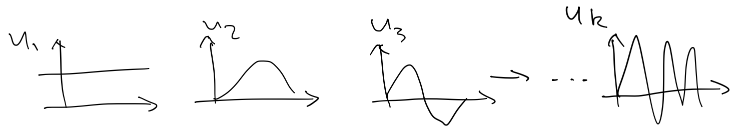
→ decreases to zero

} $\boxed{\text{rank is hard to define}}$

[cf : rank deficient : clear gap. A^+ OK then ?]

Also : singular vectors 'oscillate' more (sign changes in elements) for smaller values

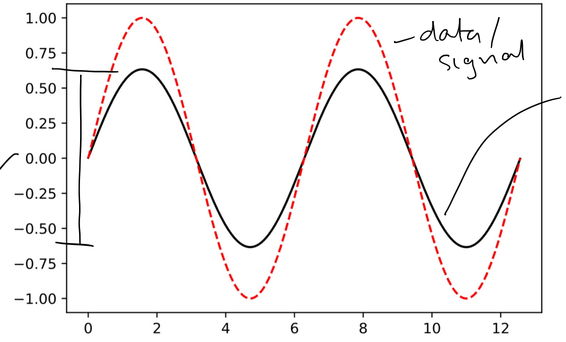
↳ Like Fourier bases (see ex.)



Example

Return to deconvolution example from L1.

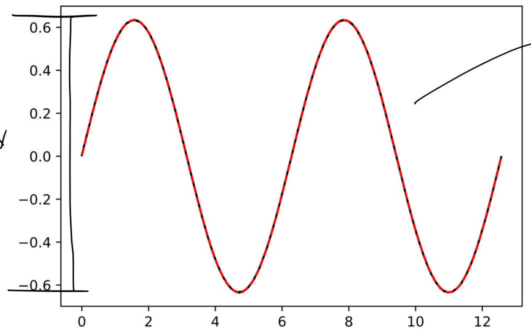
(convolution $\simeq$ window averaging
deconvolution $\simeq$ -- undoing ↑ !)



— data / signal

smoothed ("convolved") signal

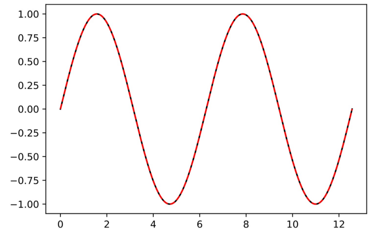
$Ax + \epsilon$



smoothed signal + tiny noise

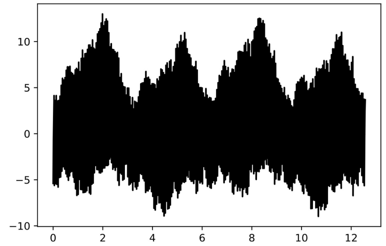
Example

Deconvolution no noise



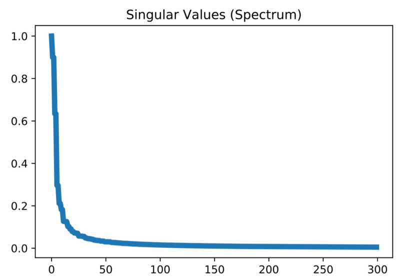
yay !

Deconvolution with noise

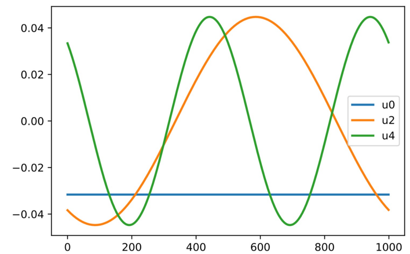


noo !

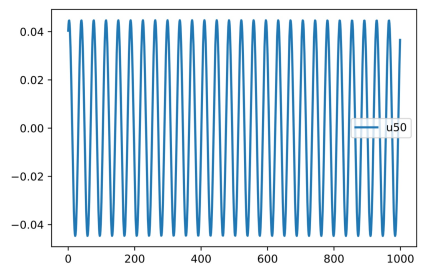
SVD : spectrum



u vectors (v similarly)



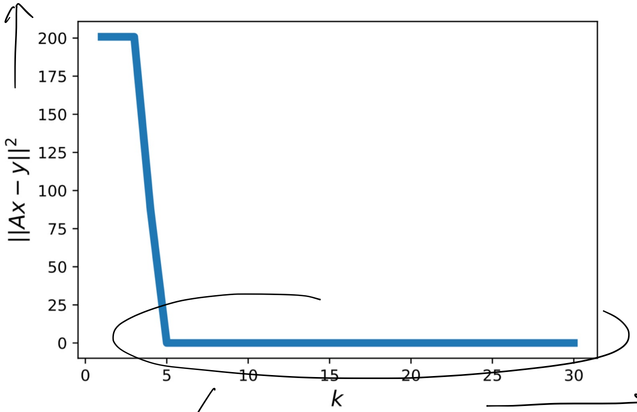
u vector for small σ_i :



Think : Fourier Components.

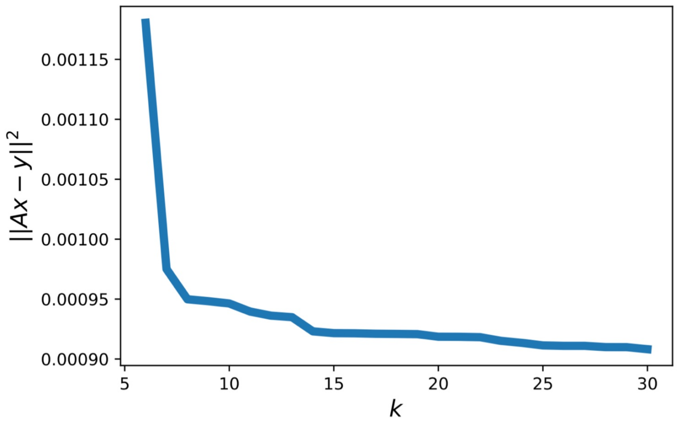
Pareto (trade-off) curve:

Fit ↑



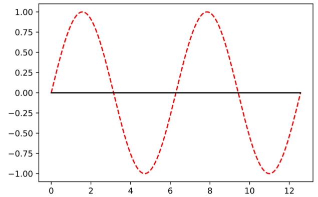
zoom

(number of retained singular values)



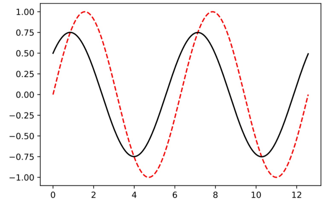
Solutions as depending on k (number retained singular values)

Stable/ Biased

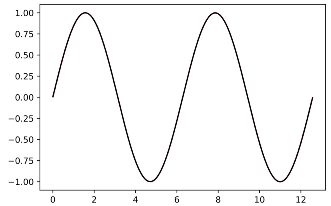


k = 1

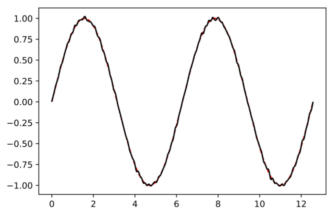
— recovered
- - - true



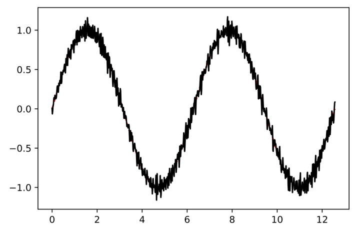
k = 4



k = 5 ← sweet spot



k = 100



k = 300

Unstable/ Unbiased

(this is a very smooth problem... typically much worse, faster)

Choosing truncation ?

Pareto :

Smallest number of singular values giving adequate fit, beyond which 'flattens'

Picard condition

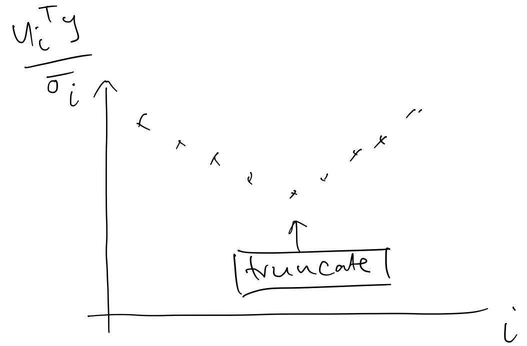
Consider

$$x = \text{Sum}\left[\underbrace{\left(\frac{u_i^T y}{\sigma_i}\right)}_{\text{coeff.}} \underbrace{v_i}_{\text{model basis}} \right]$$

Plot $\dfrac{u_i^T y}{\sigma_i}$ vs i [exercise : do for convolution!]

Expect : $u_i^T y$ decay faster initially, then start to increase

→ truncate here ↑



Note: relative decay is what matters, not abs. magnitude

Tikhonov & SVD

Finally, lets return to Tikhonov regularisation & see if SVD can help understand.

Zeroth order : Normal eq^ns

instead of λ to simplify

$$\boxed{(A^T A + \alpha^2 I)\,x = A^T y}$$

where now

$$A = U \Sigma V^T = U_r \Sigma_r V_r^T$$

$$A^T = V \Sigma^T U^T = V_r \Sigma_r U_r^T$$

$$A^T A = V \Sigma^T U^T U \Sigma V^T$$
$$= V \Sigma^2 V^T$$
$$= V_r \Sigma_r^2 V_r^T$$

→

... Tikhonov & SVD ...

can show

$$x = \mathrm{Sum}\left[\underbrace{\left(\frac{u_i^T y}{\sigma_i}\right)}_{\text{coeff.}} \underbrace{v_i}_{\text{model basis}} \right]$$

becomes

$$\boxed{x_\alpha = \sum_i^r \left[\left(f_i \cdot \frac{u_i^T y}{\sigma_i} \right) v_i \right]}$$

where

$$\boxed{f_i = \frac{\sigma_i^2}{\sigma_i^2 + \alpha^2}}$$

are the $\boxed{\text{filter factors}}$

Note: $\left\{ \begin{array}{l} \alpha = 0 \Rightarrow f_i = 1 \\ \sigma_i << \alpha \Rightarrow f_i \to \left(\frac{\sigma_i}{\alpha}\right)^2 \to 0 \\ \sigma_i >> \alpha \Rightarrow f_i \to 1 \end{array} \right\}$

$\Rightarrow$ $\boxed{\text{Tikhonov regularisation implements (continuous version of) truncated SVD !}}$

Bonus (not examinable)

Rank factorisation

$\to$ see Piziak & Odell (1999) on Canvas

Given $\boxed{m \times n}$ matrix A with $\boxed{\text{rank } r > 0}$

$\Rightarrow$ can write $\boxed{A = FG}$

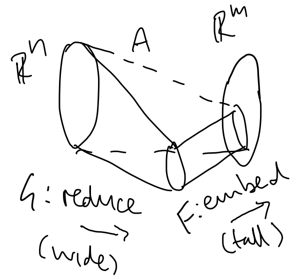
where $\boxed{\begin{array}{ll} G & r \times n \\ F & m \times r \end{array}}$

so:

$$A \sim \begin{array}{c} \\ m \end{array}\overset{r}{\begin{bmatrix} \\ \text{tall} \\ \\ \end{bmatrix}} \begin{array}{c} r \\ \\ \end{array}\overset{n}{\begin{bmatrix} \text{wide} \end{bmatrix}}$$

} note similarity to reduced SVD

ie tall $\times$ wide : $\boxed{\text{apply wide then tall}}$



idea generalises to $\boxed{\text{nonlinear}}$

$\boxed{\text{epi-mono factorisation}}$ ie $\boxed{\text{onto – 1–1 factorisation}}$

$$* \boxed{f = m \circ e} *$$

'tall' (1–1) ↑ 'wide' (onto) ↑ } nonlinear versions