# ENGSCI 741

## INVERSE PROBLEMS

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# MODULE OVERVIEW

Inverse Problems (*Oliver Maclaren*) [~9 lectures/tutorials]

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



## MODULE OVERVIEW

3. *Applications* [2-3 lectures/tutorials]
   Deblurring, numerical differentiation, parameter estimation, tomography, remote sensing...(we'll see!)



## LECTURE 5: 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 741 : Lecture 5.

Regularisation in linear problems:
The Singular Value Decomposition perspective

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- SVD
  - ∟ extension of eigen analysis
  - ∟ insight/calculation for inverses, resolution, effect of regularis.
  - ∟ the 'crown jewel' of linear algebra

- Truncated SVD.
  - ∟ as regularisation scheme.
  - ∟ connection to Tikhonov.

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## Eigenvalues

Recall that for a square matrix $A$, eigenvalues solve

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

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

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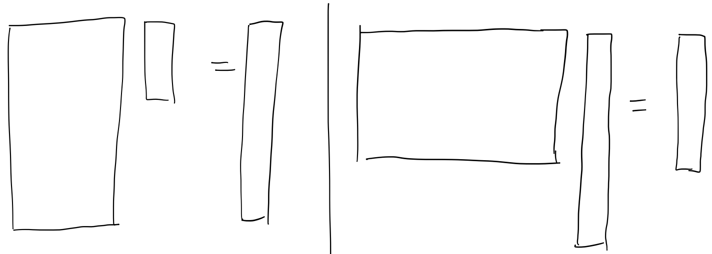

| Tall/overdetermined systems | Wide/underdetermined systems |
|---|---|
| – 'classical statistics' | – 'inverse problems'<br>– 'nonparametric statistics<br>– 'machine learning'<br>etc |

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

## Eigenvalues?

$$\left.\begin{array}{ll} A & m\times n \\ x & n \\ y & m \end{array}\right] \quad Ax = y$$

---

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

} live in different spaces!

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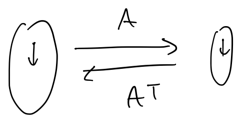
## Solutions?

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




$A^TA$: $\mathbb{R}^n \to \mathbb{R}^n$ $\quad$ $AA^T$: $\mathbb{R}^m \to \mathbb{R}^m$

## Singular values & singular vectors I.

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

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

matrix ($A$), vector ($v$), vector ($u$), scalar ($\sigma$)

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

- $u_i$: left singular vector (data space)
- $\sigma_i$: singular value
- $v_i$: right singular vector (model space)

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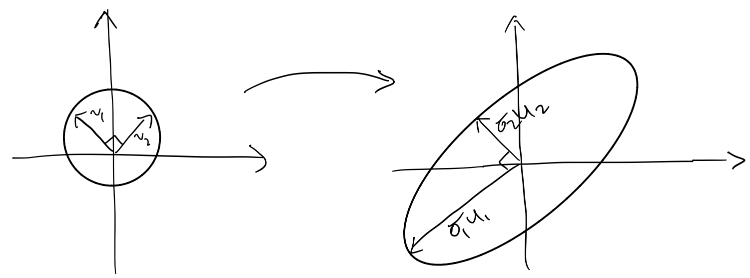


model space $\mathbb{R}^n$ $\quad x$

data space $\mathbb{R}^m$ $\quad y$

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## Singular values & singular vectors II

In particular, for singular vectors/values

$$\boxed{Av_i = u_i \sigma_i}$$

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.

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

→ generalisation to nonsquare matrices

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## Singular value decomposition (SVD) I.

Suppose for the moment all rows are independent & consider all $\boxed{Av_i = u_i \sigma_i}$ sol$^{n}$s:

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

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

→

# 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 $m \times n$

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

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# Some Properties of SVD

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

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

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

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

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

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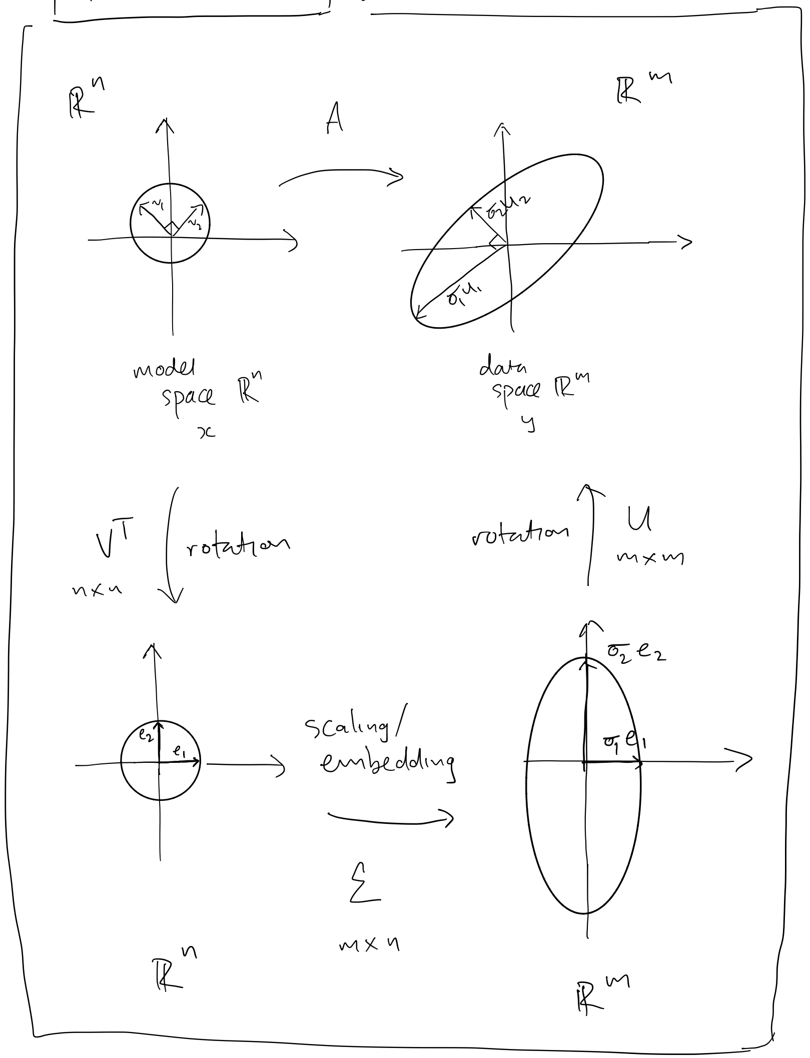
## SVD : interpretation

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




## SVD : Big picture

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

- 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.

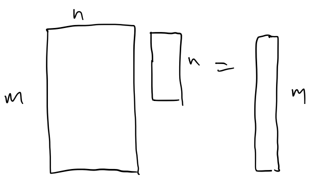
# SVD & Inverses (Left / Retraction)

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:

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

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

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

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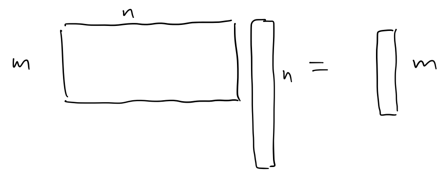
# SVD & Inverses (Right / Section)

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:

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

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

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

## 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 $V, U, \sigma$ 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)

$$R_M R_M = A^{\dagger}AA^{\dagger}A = A^{\dagger}A = R_M$$

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

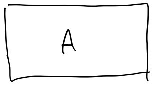
# SVD & Resolution : Explicit calculation.

Now : $\boxed{R_D = U_r U_r^T}$ $m \times m \left\{ \begin{array}{ll} U_r & m \times r \\ U_r^T & r \times m \end{array} \right.$ (r m vectors)

$\boxed{R_M = V_r V_r^T}$ $n \times n \left\{ \begin{array}{ll} V_r & n \times r \\ V_r^T & r \times n \end{array} \right.$ (r n vectors)

- If rank $\underline{r = m < n}$

  $\Rightarrow R_D = I_m$



(recover data exactly)

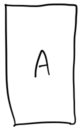
(models are 'reduced')

  But $\underline{R_M \neq I_n}$

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

  $\Rightarrow$ <u>$R_M$ is model projection operator</u>

- If rank $\underline{r = n < m}$



(data are 'reduced')

(models recovered exactly.)

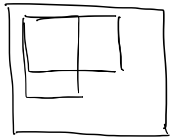
  $R_D \neq I_m$

  $\underline{R_M = I_n}$

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

  $\Rightarrow$ <u>$R_D$ is data projection</u>

- if rank $\underline{r < m \;\&\; n}$



  $R_D \neq I_m$

  $\underline{R_M \neq I_n}$

  $\Rightarrow$ <u>Both</u> are projection operators.

  $(U_r^T U_r = I,\ V_r^T V_r = I$ still $)$

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## <u>Exercise</u> (Tut/Assignment) :

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

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$\longrightarrow$

## 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

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Key: inverse leads to

$\boxed{\text{dividing by small } \sigma_i \text{ values}}$

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## SVD as basis expansion:

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

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

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

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

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...)

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

$\sigma_1$: largest singular value

$\sigma_r$: smallest singular value.

## Stability : Key point

Stability (continuity modulus) of $A^+$ governed by

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

(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)

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## Spectrum

Plot of singular values in decreasing order :


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

→ no clear gap

→ decreases to zero

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

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

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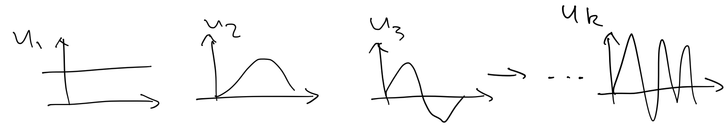
Also : singular vectors 'oscillate' more (sign changes in elements) for smaller values

↳ Like Fourier bases (see ex.)

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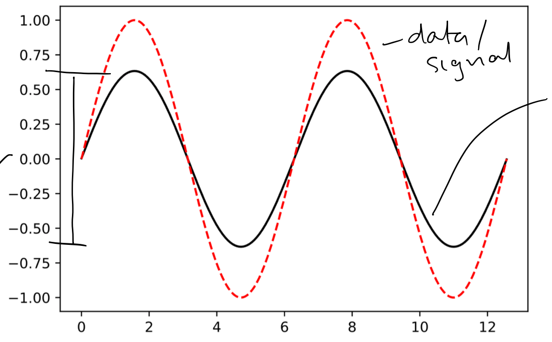
# Example

Return to deconvolution example from L1.

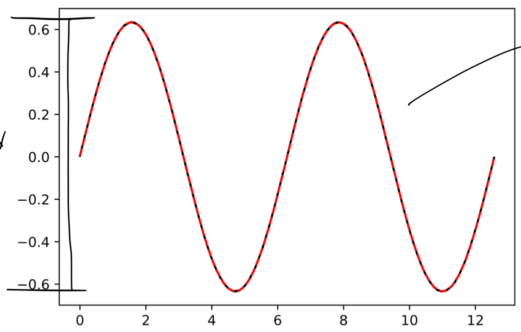
(convolution $\approx$ window averaging
deconvolution $\approx$ ..undoing ↑ ! )

$Ax + \epsilon$



data / signal

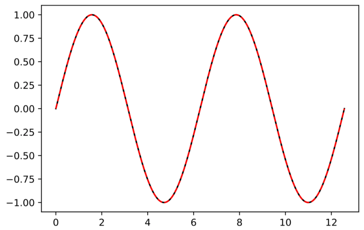
smoothed ('convolved') signal



smoothed signal + tiny noise

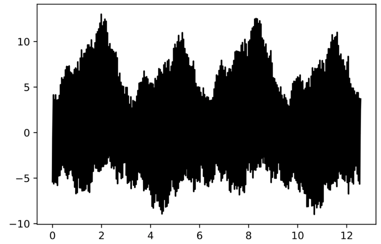
# Example

Deconvolution no noise



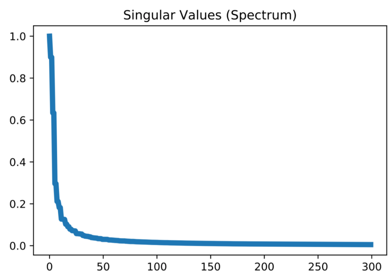
yay !

Deconvolution with noise

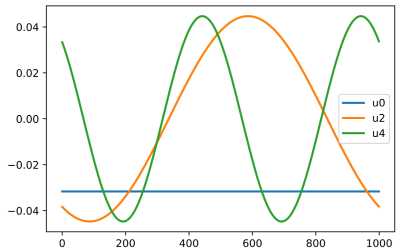


noo !

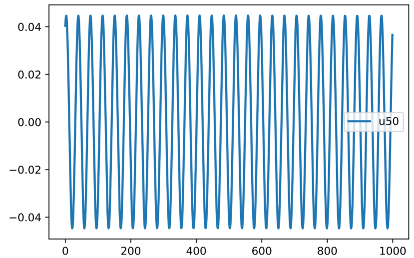
SVD : spectrum




u vectors (v similarly)



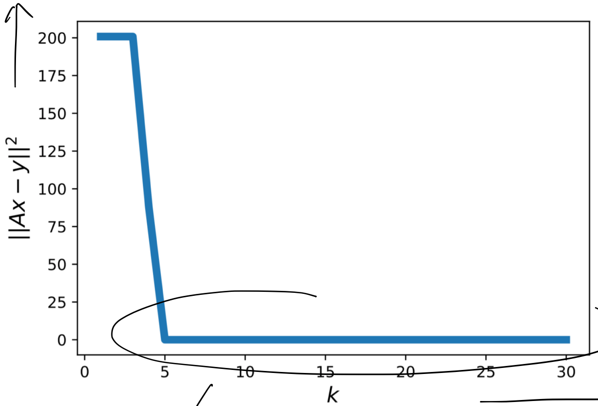

u vector for small $\sigma_i$ :




Think : Fourier components.

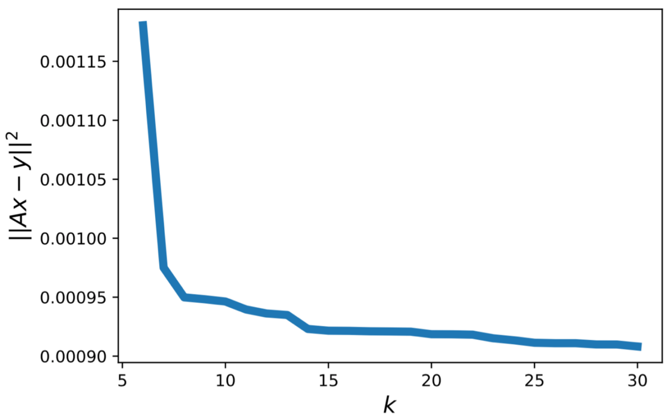
## Pareto (trade-off) curve:

Fit ↑




(number of retained singular values)

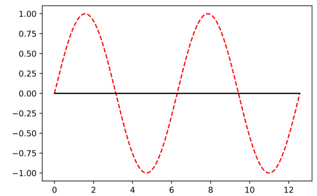
zoom



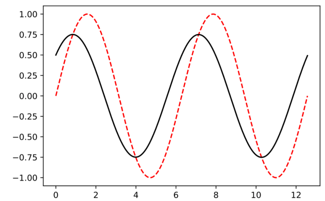

## Solutions as depending on k (number retained singular values)

— recovered
- - - true

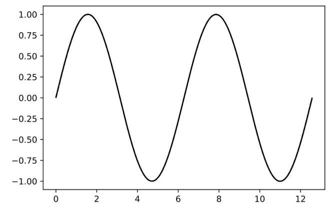
Stable/ Biased



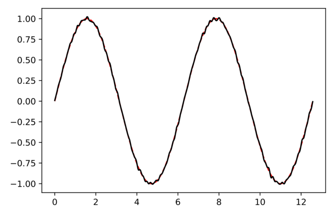
$k = 1$



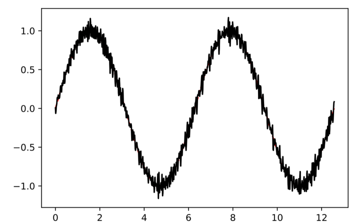
$k = 4$



$k = 5$ ← sweet spot



$k = 100$



$k = 300$

Unstable/ Unbiased

## Choosing truncation ?

**Pareto** :

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

**Picard condition**

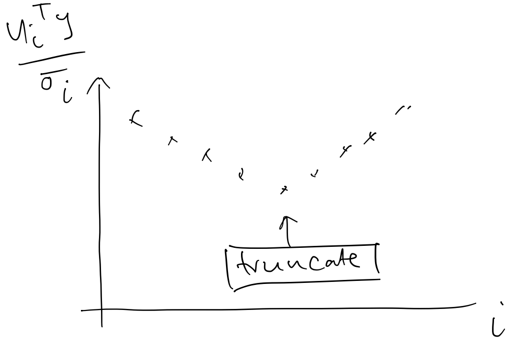
Consider

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

Plot $\frac{u_i^T y}{\sigma_i}$ 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, we lets return to Tikhonov regularisation & see if SVD can help understand.

Zeroth order : Normal eqⁿs

instead of $\lambda$ 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 filter factors

Note:

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

$\Rightarrow$ Tikhonov regularisation implements truncated SVD!