Level choice in truncated total least squares

Diana Sima   Sabine Van Huffel

Department of Electrical Engineering
Katholieke Universiteit Leuven, Belgium

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HARRACHOV

Outline

Linear approximation problems

Noisy linear system $Ax \approx b$

- A is a given $m \times n$ matrix ($m \geq n$)
- b is an m-dimensional given vector

- Least Squares finds the smallest correction to b

$$\text{LS:} \quad \min_{\Delta b, x} \| \left[\Delta b \right] \|_2^2 \quad \text{s.t.} \quad Ax = b + \Delta b$$

- Total Least Squares finds the *nearest compatible system*

$$\text{TLS:} \quad \min_{\Delta A, \Delta b, x} \| \left[\Delta A \quad \Delta b \right] \|_F^2 \quad \text{s.t.} \quad (A + \Delta A)x = b + \Delta b$$

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$$\text{TLS:} \quad \min_{\Delta A, \Delta b, x} \left\| \begin{bmatrix} \Delta A & \Delta b \end{bmatrix} \right\|_F^2 \quad \text{s.t.} \;\; (A + \Delta A)x = b + \Delta b$$

Total Least Squares

Solution method: Rank reduction of $\begin{bmatrix} A & b \end{bmatrix}$ by one.

TLS is classically solved using the SVD of $\begin{bmatrix} A & b \end{bmatrix} = U\Sigma V^\top$.
$\rightsquigarrow$ the right singular vector in V corresponding to the smallest singular value gives the TLS solution $x_{\mathrm{TLS}} := -v_{1:n,n+1} \big/ v_{n+1,n+1}$.

Possible problems

- non-uniqueness: non-unique smallest singular value
- multicollinearities: linearly dependent columns in A
- non-genericity: non-existence of the solution x (*e.g.*, when b is orthogonal to the left singular subspace corresp. to smallest singular value of A)

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Ill-posed linear algebraic systems.

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- $\begin{bmatrix} A & b \end{bmatrix}$ is ill-conditioned
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Example (ilaplace)

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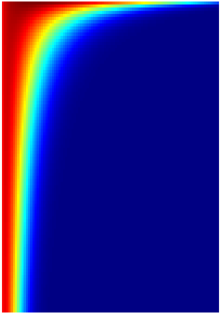
$A =$ 

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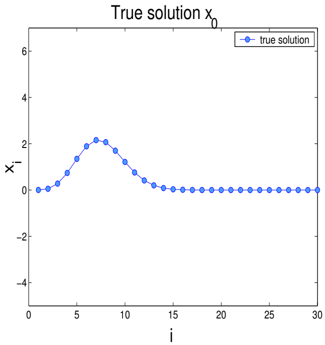

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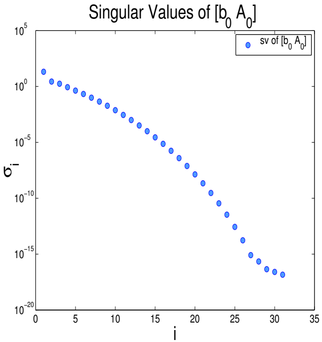

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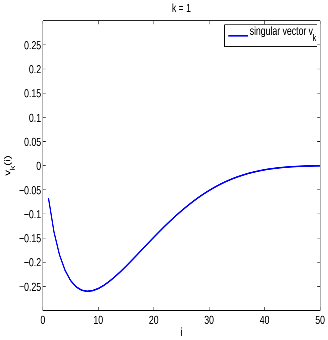

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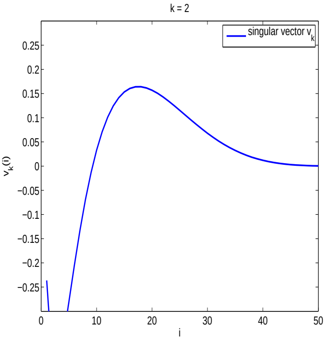

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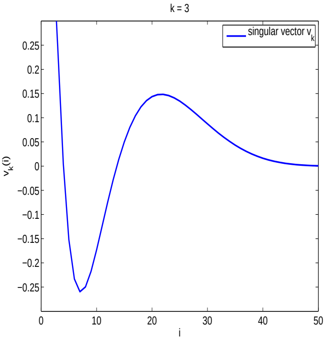

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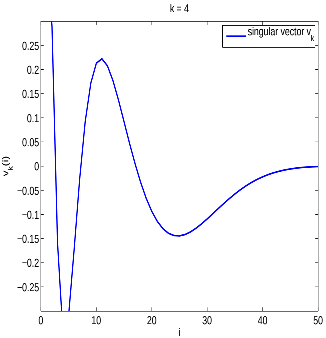

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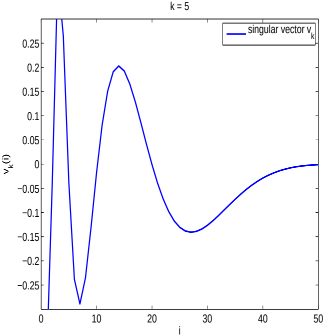

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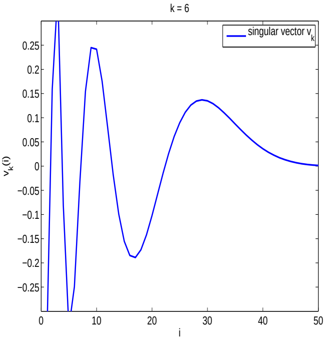

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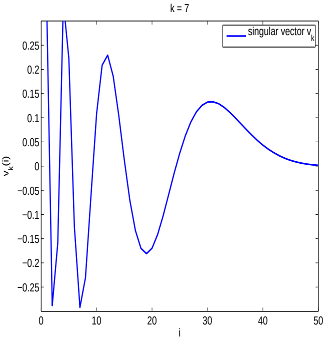

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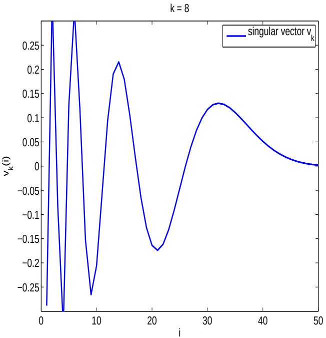

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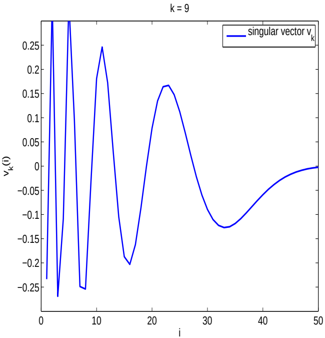

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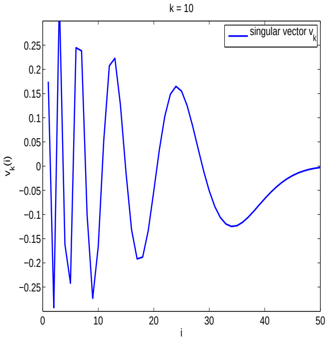

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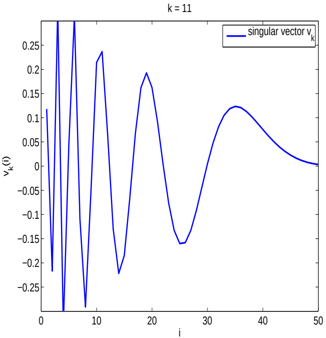

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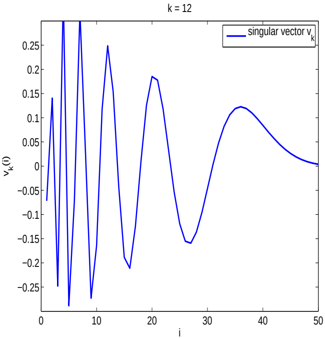

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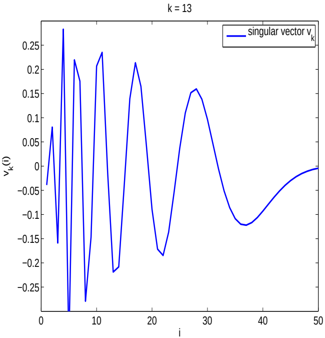

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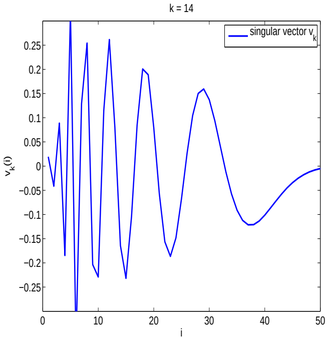

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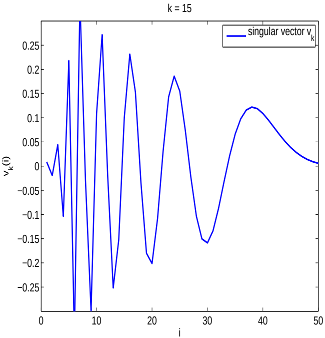

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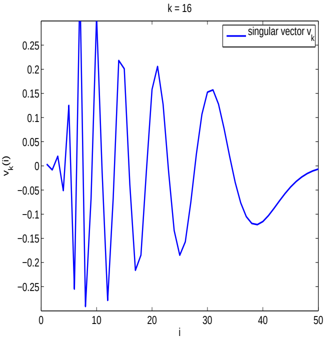

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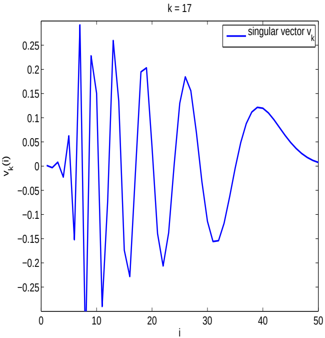

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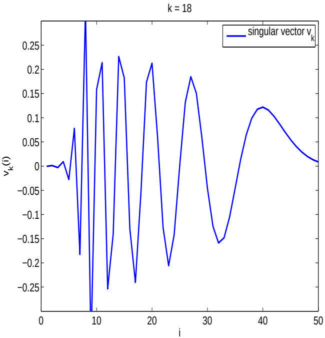

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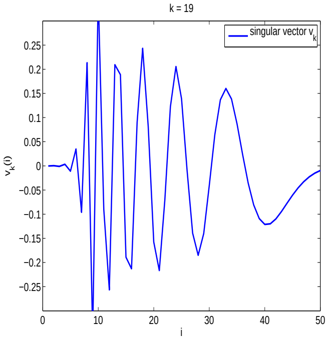

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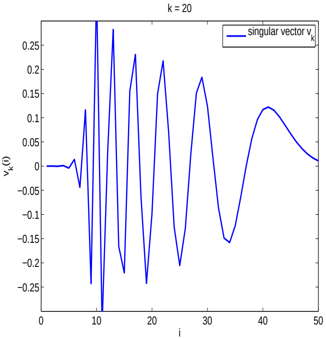

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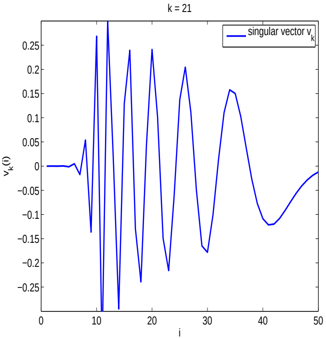

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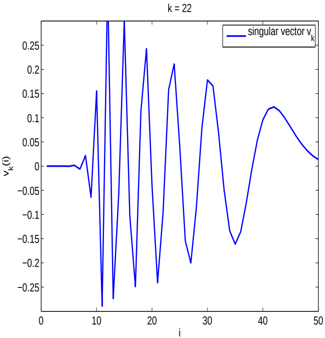

Ill-posed linear algebraic systems.

When $Ax \approx b$ originates from an ill-posed problem ...

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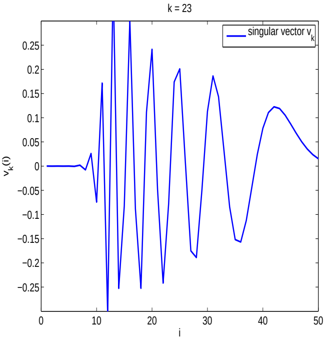

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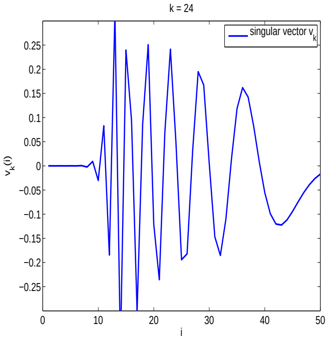

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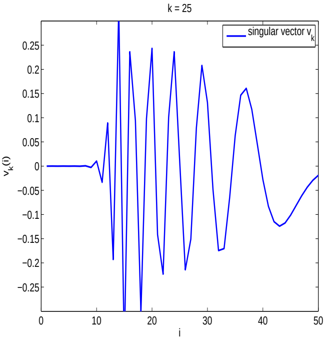

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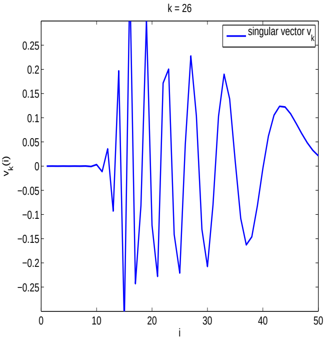

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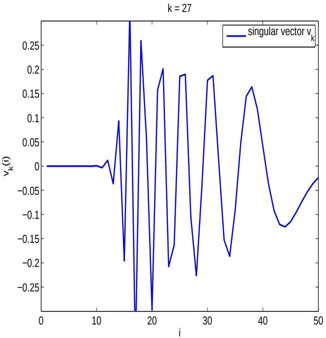

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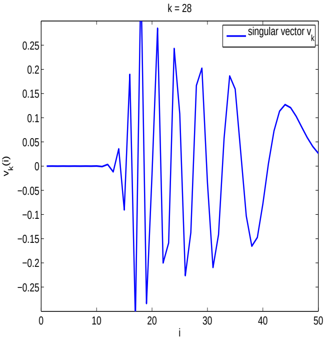

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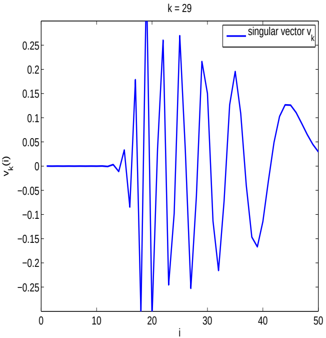

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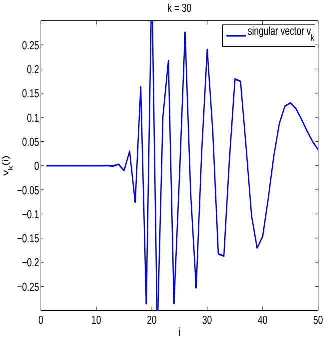

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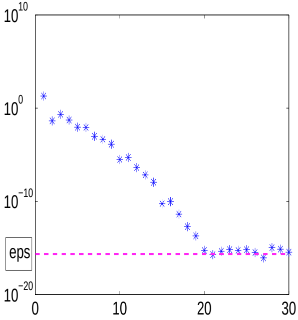


Least Squares and Total Least Squares solutions

Consider the SVDs:

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

$$\begin{bmatrix} A & b \end{bmatrix} = U\Sigma V^{\top} = \sum_{i=1}^{n+1} \sigma_i u_i v_i^{\top}$$

Least Squares solution

$$x_{\mathrm{LS}} = A^{\dagger} b = \left(A^{\top} A\right)^{-1} A^{\top} b = \sum_{i=1}^{n} \frac{u_i'^{\top} b}{\sigma_i'} v_i'$$

Total Least Squares solution

$$x_{\mathrm{TLS}} = \left(A^{\top} A - \sigma_{n+1}^2 I_n\right)^{-1} A^{\top} b = -v_{1:n,n+1} / v_{n+1,n+1}$$

x_{TLS} is a *de-regularized* LS solution.

Truncated SVD

- let $k \leq n$ be a truncation level
- compute the nearest rank k approximation of A using the SVD: $A'_k = U' {\Sigma'_k}^{\dagger} {V'}^{\top}$, with $\Sigma'_k = \text{diag}\{\sigma'_1, \ldots, \sigma'_k, \underbrace{0, \ldots, 0}_{n-k}\}$.
- solve in the LS sense the 'truncated' problem $A'_k x \approx b_k$

$$
\begin{aligned}
x_{\text{TSVD},k} &= V' {\Sigma'_k}^{\dagger} {U'}^{\top} b \\
&= \sum_{i=1}^{k} \frac{{u'_i}^{\top} b}{\sigma'_i} v'_i
\end{aligned}
$$

Truncated Total Least Squares

Truncated TLS

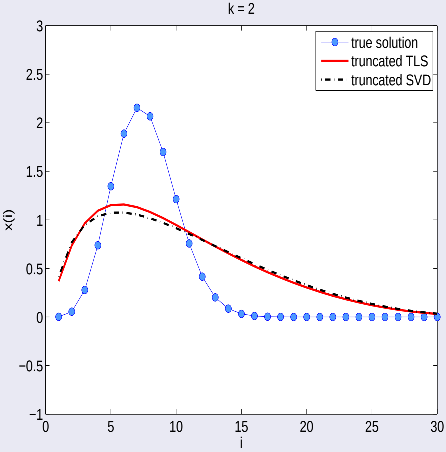
- let $k \leq n$ be a truncation level
- compute the nearest rank k approximation of $\begin{bmatrix} A & b \end{bmatrix}$, $\begin{bmatrix} A_k & b_k \end{bmatrix}$, using the SVD
- solve in the TLS sense the 'truncated' problem $A_k x \approx b_k$

$$x_{\mathrm{TTLS},k} = -V_{12}^k (V_{22}^k)^\dagger = -V_{12}^k (V_{22}^k)^\top / \|V_{22}^k\|^2,$$

where we partition V as (with $\ell = n - k + 1$):

$$V = \begin{array}{c c} \overset{k}{\longleftrightarrow} \quad \overset{\ell}{\longleftrightarrow} & \\ \begin{bmatrix} V_{11}^k & V_{12}^k \\ V_{21}^k & V_{22}^k \end{bmatrix} & \begin{matrix} \updownarrow\ n \\ \updownarrow\ 1 \end{matrix} \end{array}$$

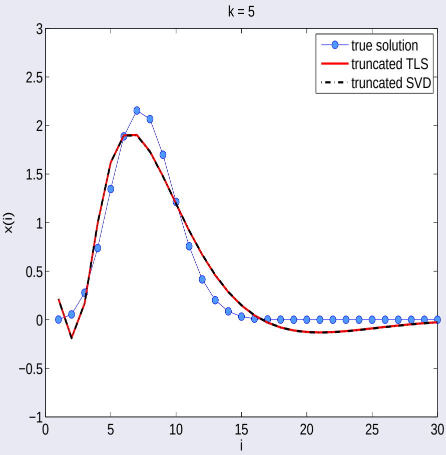
Example: effect of truncation levels



Example

The noisy ill-posed problem $Ax \approx b$.

Example: effect of truncation levels



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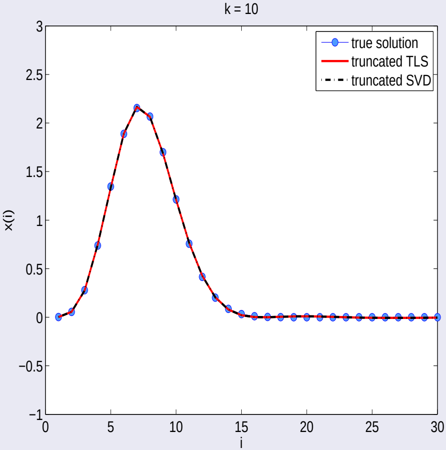

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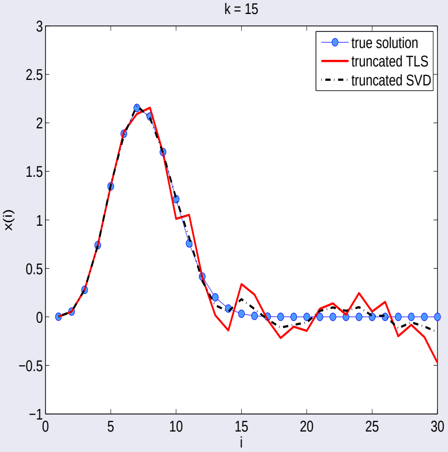

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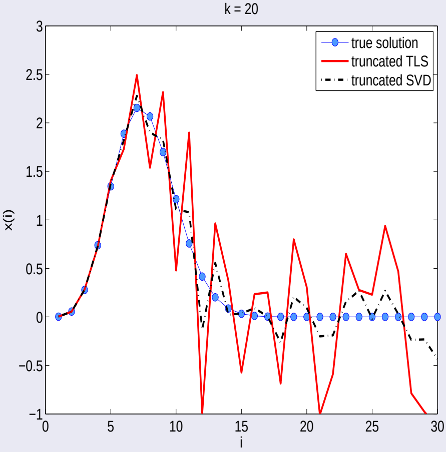

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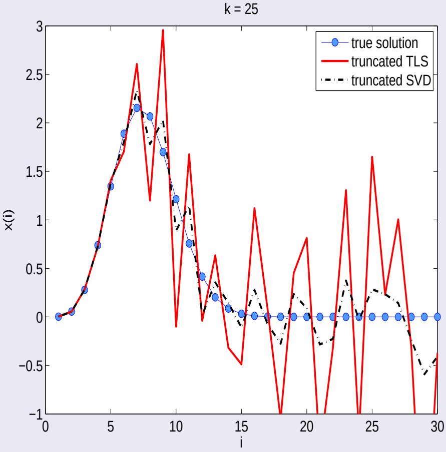

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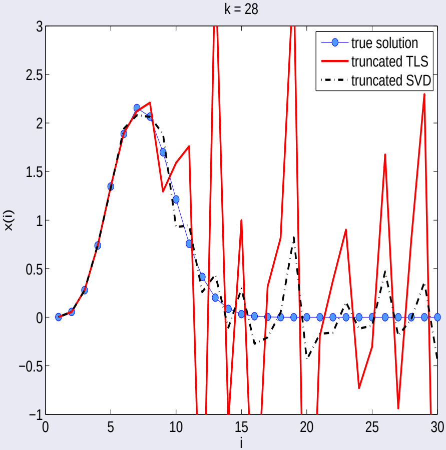

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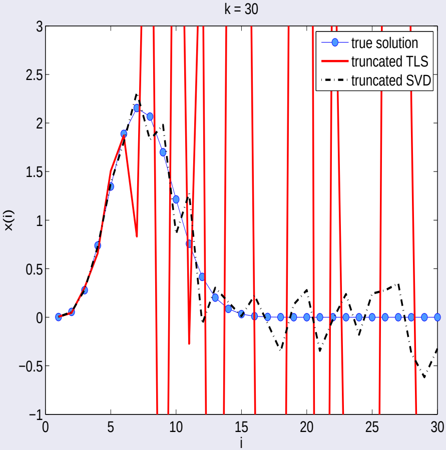

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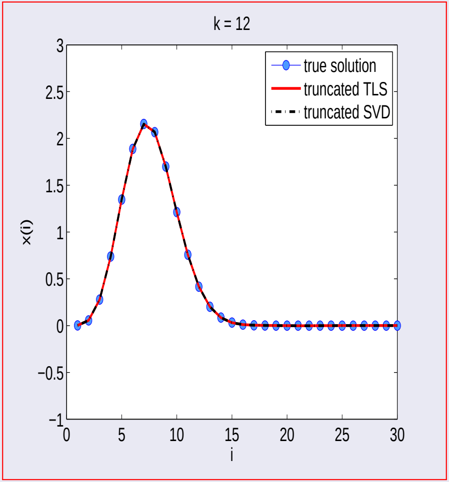

Example

The noisy ill-posed problem $Ax \approx b$.

Optimal truncation level at $k = 12$.

The filter factors for regularized solutions

The TSVD solution has a simple interpretation in terms of filter factors. If we set

$$f_1' = f_2' = \ldots = f_k' = 1, \quad \text{and} \quad f_{k+1}' = \ldots = f_n' = 0,$$

then the TSVD solution with truncation level k is simply:

$$x_{\mathrm{TSVD},k} = \sum_{i=1}^{n} f_i' \frac{u_i'^{\top} b}{\sigma_i'} v_i',$$

In general, a regularized solution to $Ax \approx b$ can be written as

$$x^{\mathrm{reg}} = \sum_{i=1}^{n} f_i \frac{u_i'^{\top} b}{\sigma_i'} v_i',$$

with $f_i \in [0, 1]$.

The TTLS filter factors

Fierro *et al.* (1997): filter factors for the TTLS solution $x_{\text{TTLS},k}$

$$f_i^k = \sum_{\substack{j=k+1 \\ \sigma_j \neq \sigma_i'}}^{n+1} \frac{v_{n+1,j}^2}{\| V_{22}^k \|^2} \left(\frac{\sigma_i'^2}{\sigma_i'^2 - \sigma_j^2} \right), \qquad i = 1, \ldots, n,$$

Properties of the TTLS filter factors:

- the first k filter factors f_i^k form a monotonically increasing sequence and satisfy

$$i = 1, \ldots, k$$

- the last $n-k$ filter factors satisfy

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$$1 + \frac{\sigma_{n+1}^2}{\sigma_i'^2 - \sigma_{n+1}^2} \leq \; f_i^k \leq 1 + \frac{\sigma_{k+1}^2}{\sigma_i'^2 - \sigma_{k+1}^2} \qquad i = 1, \ldots, k$$

- the last $n-k$ filter factors satisfy

$$\frac{\|V_{21}^k\|^2}{\|V_{22}^k\|^2} \left(\frac{\sigma_i'^2}{\sigma_1^2 - \sigma_i'^2} \right) \leq \; f_i^k \leq \|V_{22}^k\|^{-2} \frac{\sigma_i'^2}{\sigma_k^2 - \sigma_i'^2} \qquad i = k+1, \ldots, n$$

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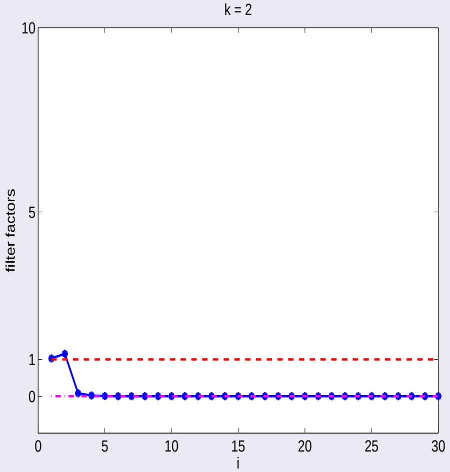
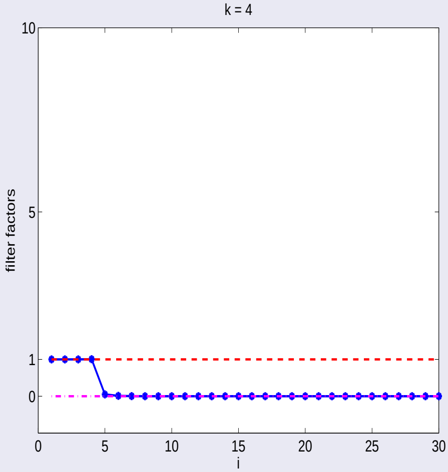


Example

The filter factors for TTLS: $f_1^k, \ldots, f_n^k$.
For too large truncation levels, the filter factors increase dramatically above 1.



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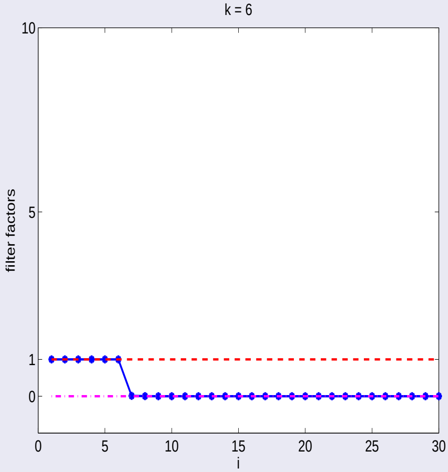

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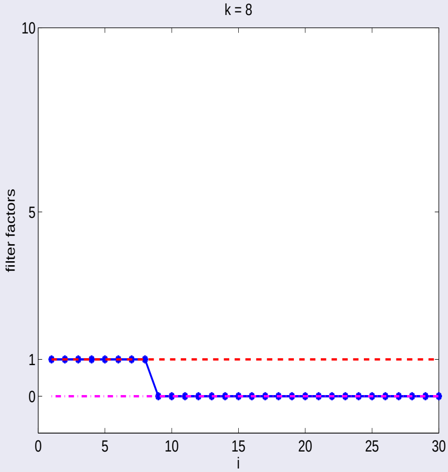

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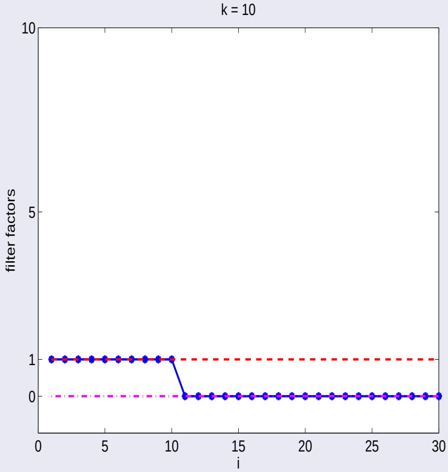

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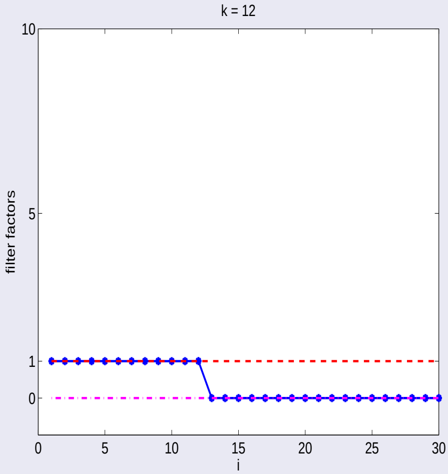

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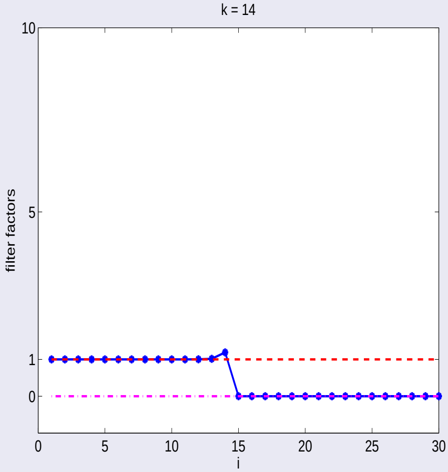

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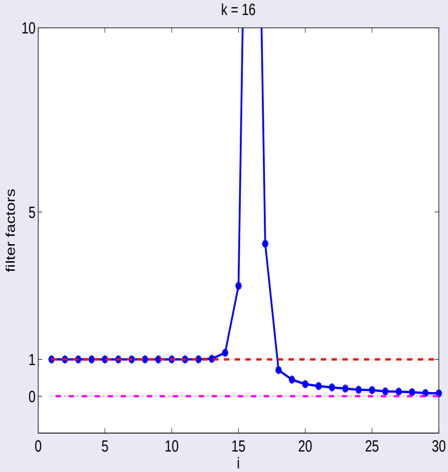

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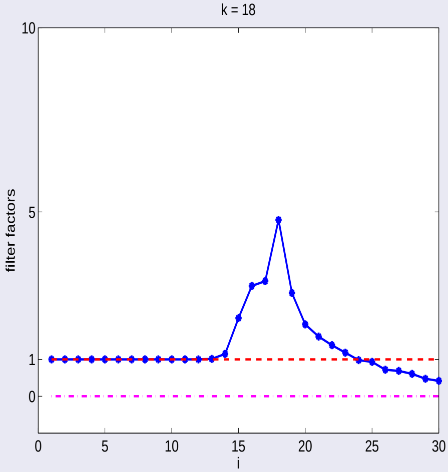

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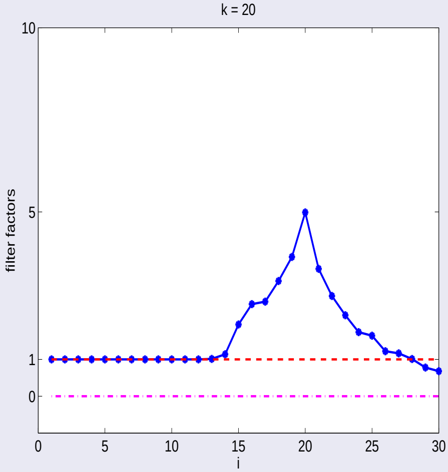

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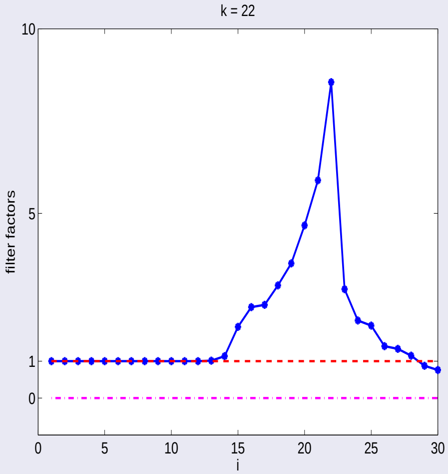

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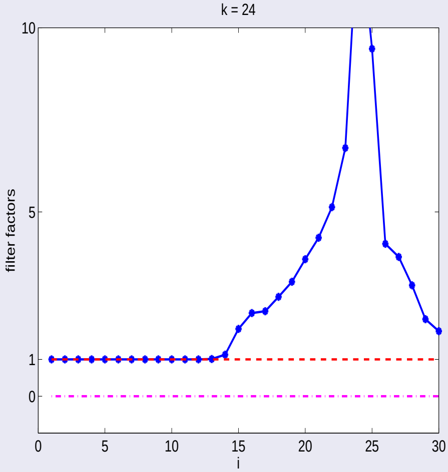

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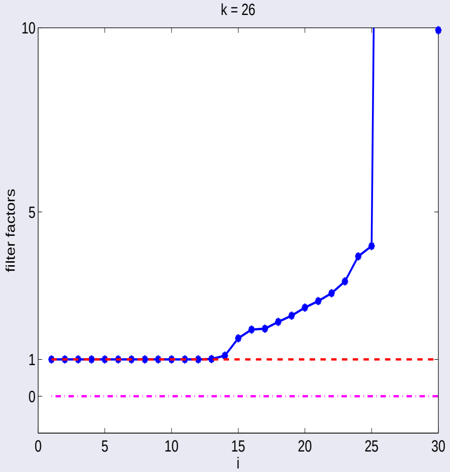

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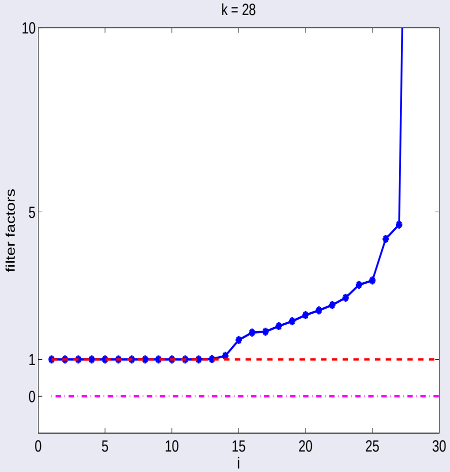

Example

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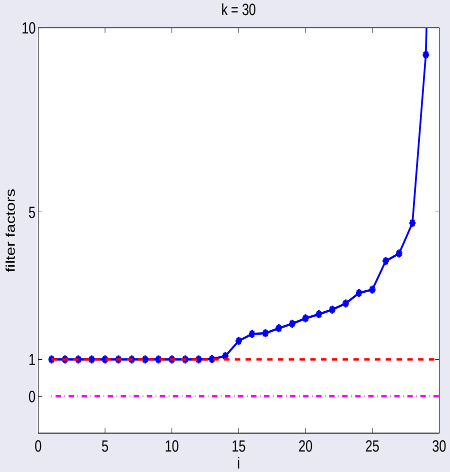
The TTLS filter factors



Example

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Choosing the truncation level

Generalized Cross Validation (GCV)

- GCV for TSVD:

$$\min_k \frac{\|Ax_{\text{TSVD},k} - b\|^2}{(m-k)^2}$$

- GCV for TTLS:

$$\min_k \frac{\|Ax_{\text{TSVD},k} - b\|^2}{(m-p_k^{\text{eff}})^2},$$

where $p_k^{\text{eff}} = \sum_{i=1}^{n} f_i^k$ = effective number of parameters.

$p_k^{\text{eff}} \gg k \Longrightarrow$ the GCV function for TTLS has a better defined minimum compared to the GCV function for TSVD

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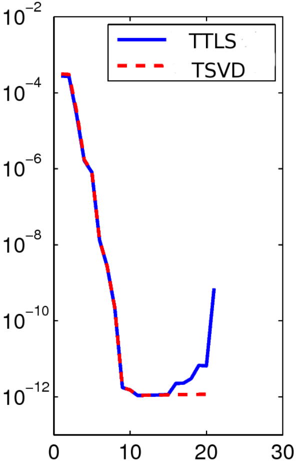
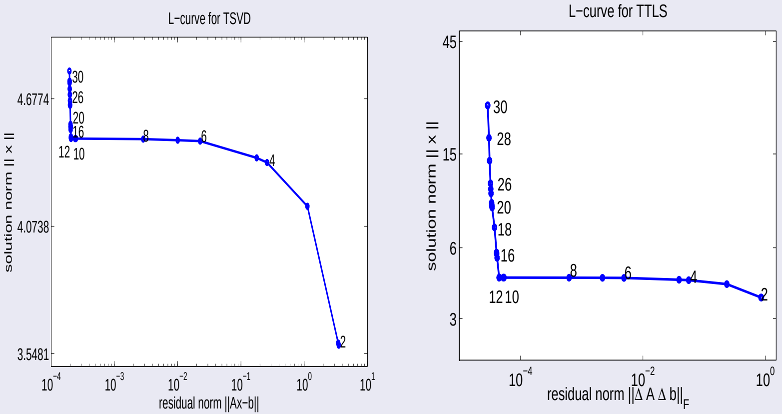


Choosing the truncation level

L-Curve

- the norm of truncated solution $||x_k||_2$ is plotted against norm of residual error for various k's
- the k corresponding to the *corner* is chosen

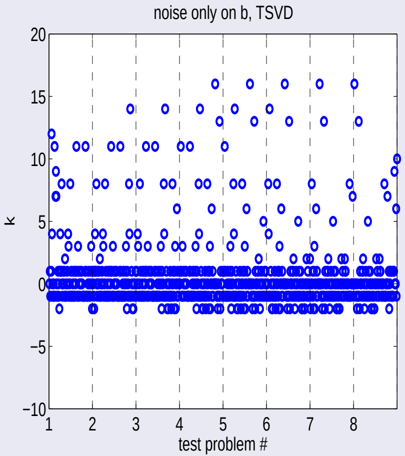
L-Curve


L−curve for TSVD
solution norm || x ||
residual norm ||Ax−b||
4.6774
4.0738
3.5481
30
26
20
16
12
10
8
6
4
2
L−curve for TTLS
solution norm || x ||
residual norm ||Δ A Δ b||F
45
15
6
3
30
28
26
20
18
16
12
10
8
6
4
2

Comparison of GCV-TSVD and GCV-TTLS

Best truncation level defined as: $\arg\min_k \|x_{\text{trunc},k} - x_{\text{true}}\|$

Estimated truncation level minus best truncation level



8 examples from the Regularization Tools:

1. `ilaplace(n,1)`
2. `ilaplace(n,3)`
3. `baart`
4. `shaw`
5. `phillips`
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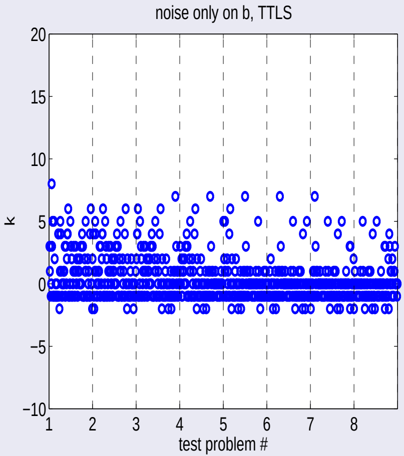

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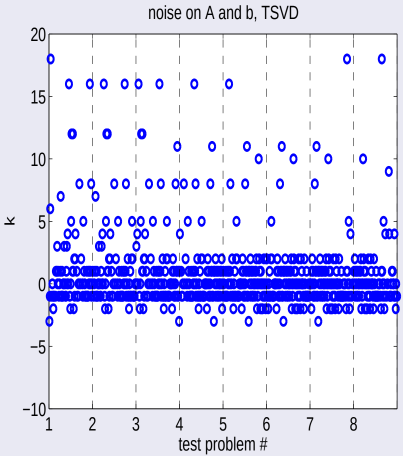

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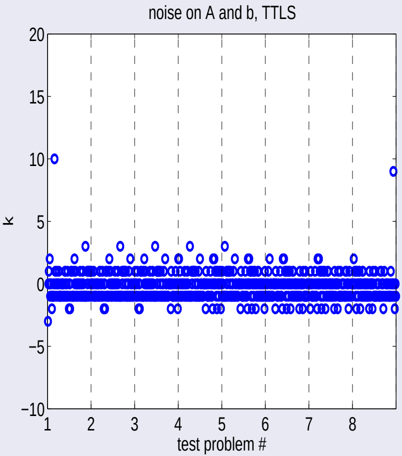

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Summary

- Truncated Total Least Squares—an alternative to Truncated SVD for discrete ill-posed linear systems
- good truncation levels are more easily identified in the context of Truncated Total Least Squares

R. D. Fierro, G. H. Golub, P. C. Hansen and D. P. O'Leary (1997) "Regularization by truncated total least squares", *SIAM J. Sci. Comput.* 18.

D.M. Sima and Sabine Van Huffel (2007) "Level choice in truncated total least squares", *Comp. Stat. & Data Anal.* (to appear).

Thank you for your attention!